Micro and Nanoscale Energy Transport
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Lecture – 25
Derivation of Continuum Laws from
Boltzmann Transport Equation Part 2

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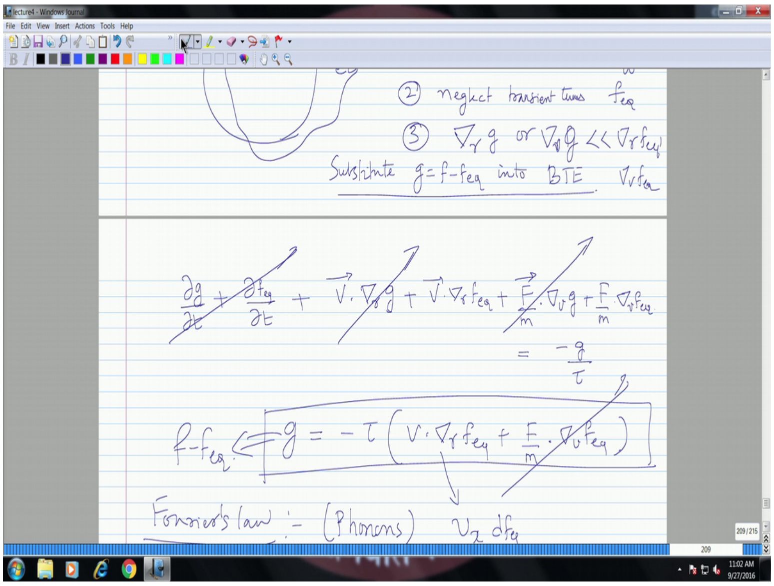

We will continue our discussion related to the Transport Phenomena. So, in the last class I hope you recall it is been quite some time now you recall the assumptions that we made in order to derive the equilibrium constitute laws.

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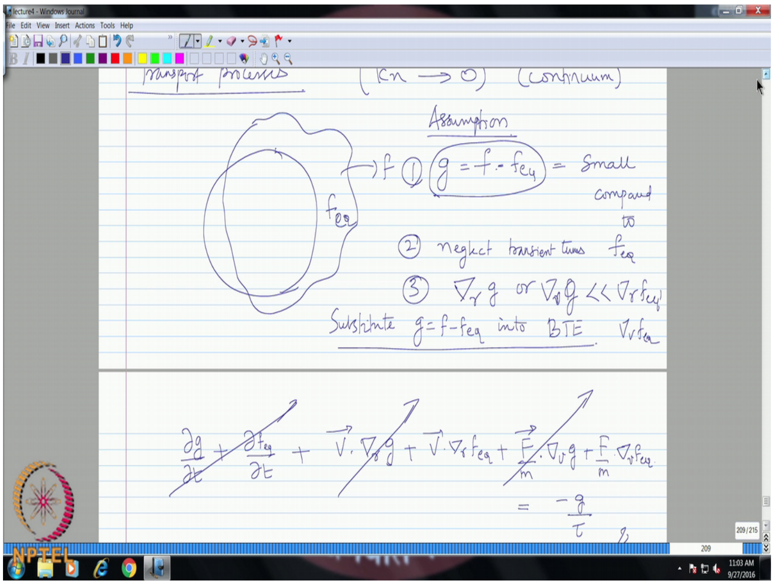

Basically, we have to start from the non Equilibrium Distribution Function. But the fact here is since, we are deriving continuum laws we can make some approximations. One of that is the deviation from the equilibrium distribution function is quite small that. So, that is in one way when, you look at the quantity t by tau if your relaxation time is quite small; that means, this t by tau is quite large which means that the non equilibrium will quickly relax to the equilibrium or deviation between f minus f naught will be very small because f minus f naught is proportional to e power minus t by tau.

Therefore, when you are looking continuum, you can make safely this assumption that f, f minus, f naught is quite small and we are calling this by another distribution function g which measures the deviation from the equilibrium and we assume that, this is small compared to f equilibrium itself apart from that; also we have to make sure the gradient or derivatives of g in spatial direction or momentum plane. So, should be smaller compared to the corresponding derivatives of equilibrium distribution function, so with these assumptions when we substitute for f in terms of g and f equilibrium into the BTE and we can knock off certain terms including the unsteady terms. So, we can assume that to derive the constitutive laws you do not have to consider transient process.

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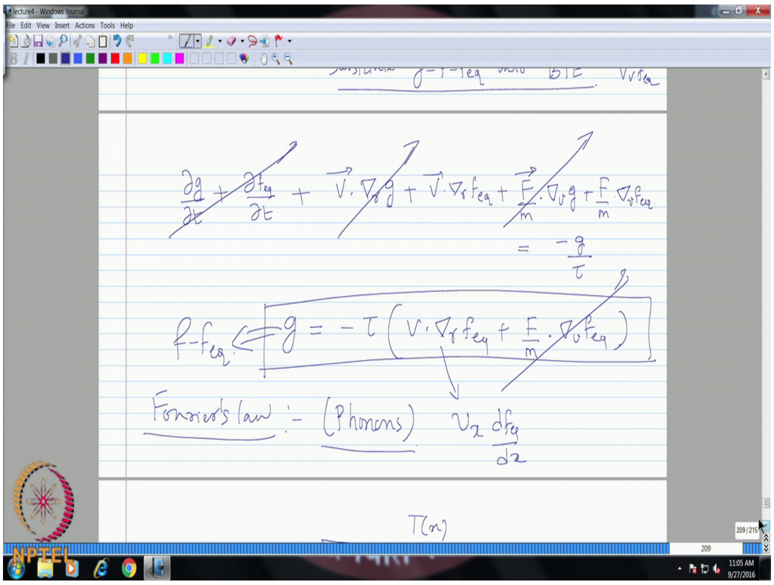

So, just a steady state should be sufficient and also with these assumptions you end up with the reduced form of the Boltzmann Transport Equation, which connects you are a non equilibrium distribution function as a function of f equilibrium. Now, we can start applying this to different systems. So, first if you want to apply this to phonons, we can derive the Fourier’s law. Therefore in the case of phonon transport it is only transporting heat and there is no electric field or external forces acting on the energy carriers. Therefore, the change in momentum will be 0. So, we can neglect the derivatives with respect to the momentum plane and therefore, we have only one derivative in the physical space which is actually you can express in terms of a spherical coordinate system. Now, we consider one dimensional transport of heat and we can write down the expression for heat flux along the positive x direction.

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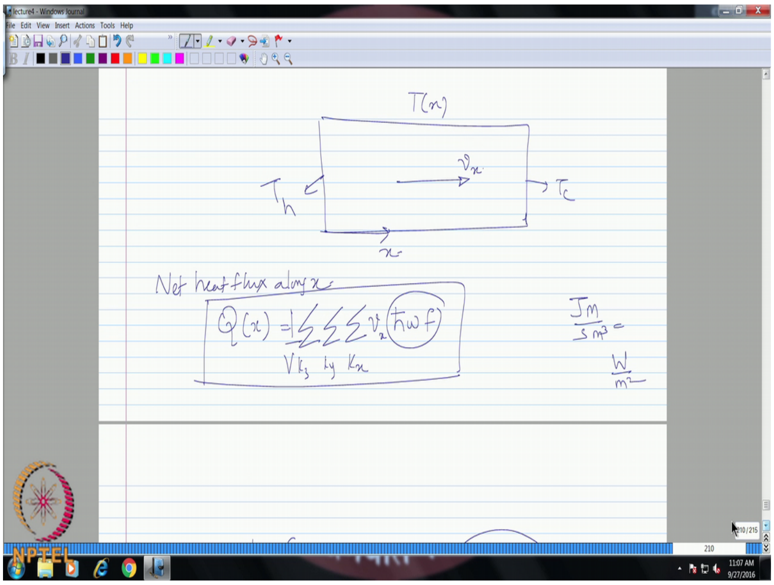

Suppose; what your non Equilibrium Distribution Function is, and the energy of each quantum state h bar omega. So, we can calculate the heat flux as a corresponding energy times the velocity in that particular direction and we can therefore, this will be the component of energy flux for one quantum state. So, we can sum this over all the quantum states k x ky k z and divided by the volume to get the unit is of heat flux watt per meter square right. So, this is similar to the statistical equilibrium case except there, we were finding out the internal energy and we were just doing the summation over all the quantum states and we use h bar omega time's f equilibrium there. Now, for the flux we have to also consider not equilibrium, but non equilibrium distribution and multiply by the corresponding velocity.

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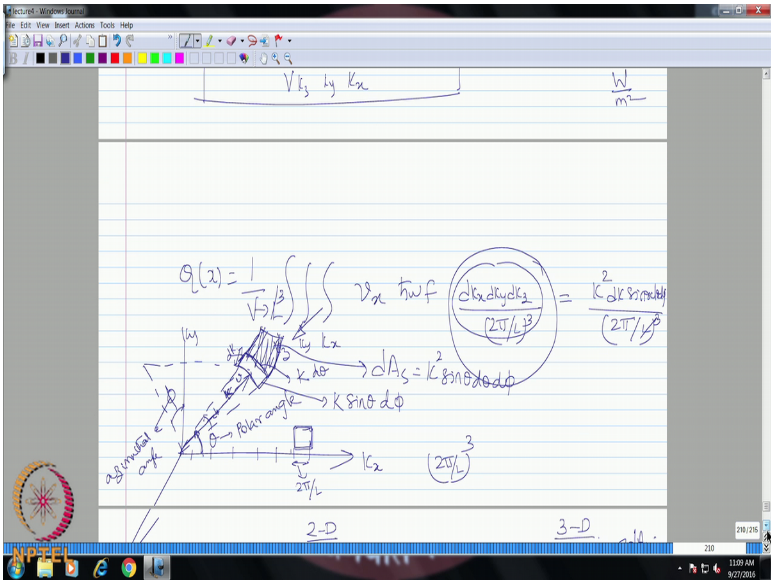

So, this is the basic principle from which now we go on further the mathematical details which include conversion from the discrete summation into an integral function and to do this. We now resolve the quantum states into a three dimensional spherical coordinate system. So, these discrete quantum states are supposed to be contained within a huge sphere. The spheres of radius from going from 0 to infinity, few solid sphere, and therefore, if you take one solid angle subtend the area that is subtended by the solid angle. So, we can write down the corresponding relation between the area or the volume and the corresponding d k x d k y d d k z and when we do this conversion. So, I think we already did those things in the last class.

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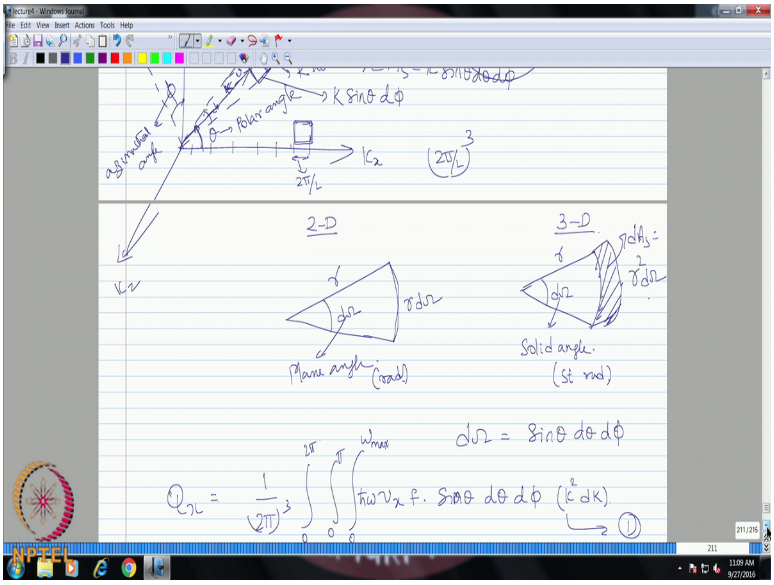

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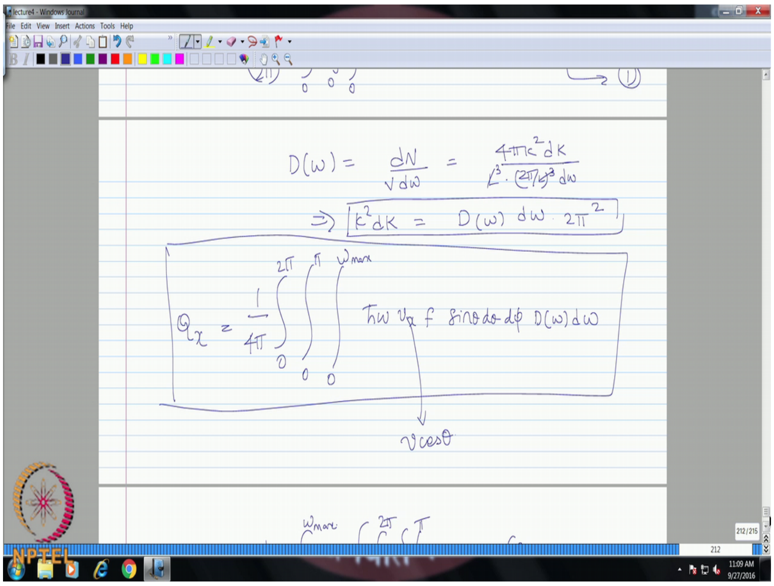

So, we can finally, write down in terms of quantum states we can replace them in terms os density of states and which now looks something like this. Therefore, we started from a discrete summation over all the quantum states we replace that with a integral over all the quantum state sphere, spherical coordinate system and from there we use the concept of density of states to convert the momentum k into the energy or frequency omega and finally, therefore we have converted the k space or the momentum space into a physical coordinate space this is subtended by a sphere and the corresponding frequency space. Therefore, we have three integrals here in place of k x ky kz. So, 2 integrals one with respect to the um the polar angle theta going from 0 to pi and the other is the Azimuthal angle 0 to 2 pi. So, this will make us complete sphere and the third integral is over the entire frequency space. So, 0 to omega max.

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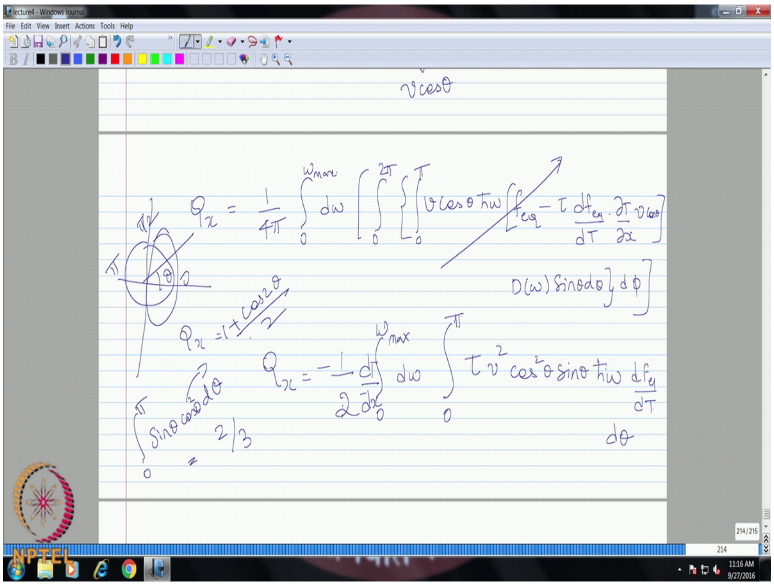

So, these are all the finer mathematical details and from this point, we know substitute for the expression for non equilibrium distribution function f which we have now written in terms of f equilibrium. Therefore, now this is going to be much easier to integrate since; everything is in terms of f equilibrium. Therefore, finally, we reach this particular expression here, now what will be the integral 0 to pi v times cos theta into f equilibrium into sine theta d theta and again integrate 0 to 2 pi d phi say, f equilibrium is actually uniform over theta and phi.

So, it does not change with respect to theta and phi f equilibrium is only a function of temperature. If you take the Bohr's Einstein distribution function it is a function of what omega and temperature. So, it there is no dependency on therefore directional space. So, it is uniform over the entire direction that is why I plotted f equilibrium as something like this it is uniform. Therefore, when you have a uniform distribution and you integrate you multiply that with cos theta. Therefore, what happens about the y axis this is going to be? So, this part is going to be cos theta will be? So, totally it will be 0. So, f equilibrium cos theta on this side, this is from let us say 0 to pi by 2 and this is from pi by 2 to pi. So, our definition of theta is this correct.

Therefore, when we say cos 0 to pi by 2, in that it will be positive pi by 2 to pi it will be negative and it will be symmetrical about the central line, therefore, if you multiply f equilibrium cos theta. So, this is going to be 0 to pi it will become 0. Therefore, this entire term this f equilibrium entire term will vanish understand is that clear. So, f equilibrium is constant here independent of theta and phi. Therefore, if you just say integral cos theta from 0 to pi. So, 0 to pi by 2 is positive pi by 2 to pi is exactly negative the same magnitude. So, this will be just dropping off.

So, it will be 0 and therefore, we end up with simply 1 by 4 pi 0 to omega max we have d omega and 0 to pi. So, we have tau into i. Therefore, this terms going to go away we have v into v v square and we also have cos square theta sine theta d theta we also have h bar omega and we also have this term right here which is d f equilibrium by dt and dt by dx can now be pulled out of the integral, we can write this outside here as dt by dx. This is independent of your directional space and frequency or for a particular case we maintain temperature difference.

So, then this is therefore, d theta here and when you integrate d phi. So, the dependence 0 to 2 pi d phi is just 2 pi right. Therefore, this becomes 1 over 2. So, 2 pi in the numerator and four pi in the denominator this becomes 1 over 2 till that clear is that. Now, we have integrals in terms of theta and omega. So, you can evaluate this integral with respect to theta. So, that is basically 0 to pi sine theta cos square theta d theta this is what you have to evaluate and if you do this you will get this is equal to 2 by 3. So, you to use cos square theta is one plus cos 2 theta by 2 into this and then, we will be able to find out this integral.

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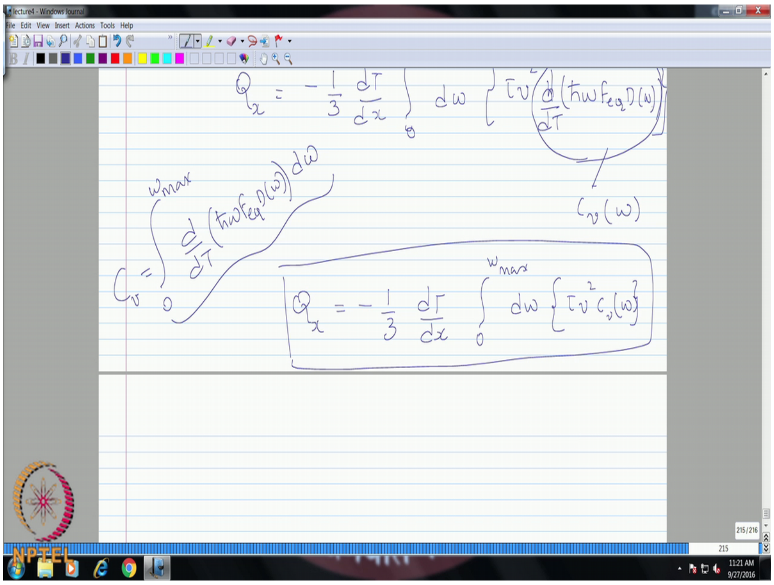

Therefore, your Q x will become minus 1 by 3 dt by dx 0 to omega max d omega tau v square. Now I can take h bar omega just inside this term d by dt I can write this as h bar omega f equilibrium into d omega i-i missed d omega here, there should be d omega here this is your density of states. Therefore, now anybody recollect what is this? I think you should be able to recollect.

Student: (Refer Time: 14:50).

So, this is your polymeric heat capacity is that ok? You go back and check. So, the simplest thing h bar omega into f equilibrium what is that?

Student: Energy minus.

Energy of a single quantum state.

Therefore, integrate it from 0 to omega max h bar omega f f equilibrium d d of omega that will give you the internal energy total internal energy for that entire system. So, du by dt will be your volumetric heat capacity. Therefore, here what we have written d by dt of h bar omega f equilibrium d omega is the volumetric heat capacity of a single quantum state a single frequency, if is the integrated over all the frequency that will be the total volumetric heat capacity, understand? Therefore, this is nothing, but we can write this is c v within bracket omega.

So, this is this is a micro again a micro state heat capacity you understand? If you integrate this over all the micro states that will give you the macro state heat capacity. Therefore, why I am doing this is because this is a function of frequency. So, and you get tau and v also tau for example, could also be a function of frequency. So, we cannot simply assume tau and v as constant and take them out and then, simply write this as c we can sometimes do that for special cases for generic cases the relaxation time is also a function of frequency.

Because if you go back and see the different kinds of scattering mechanisms you have talked about phonon scattering, so for example, the Umklapp scattering is a function of frequency and same way the impurity phonon impurity scatterings right that is similar to a relays scattering. So, function of frequency to the power 4. Therefore, in all these cases tau is also a function of frequency and we cannot simply assume this to be a constant. Therefore, we can write this as 1 by 3 dt by dx 0 to omega max d omega tau v square c omega.

So, this is your final expression and so, this is your Fourier’s law in fact, if how to identify the expression for conductivity this is there Fourier’s law, so where conductivity k will be.

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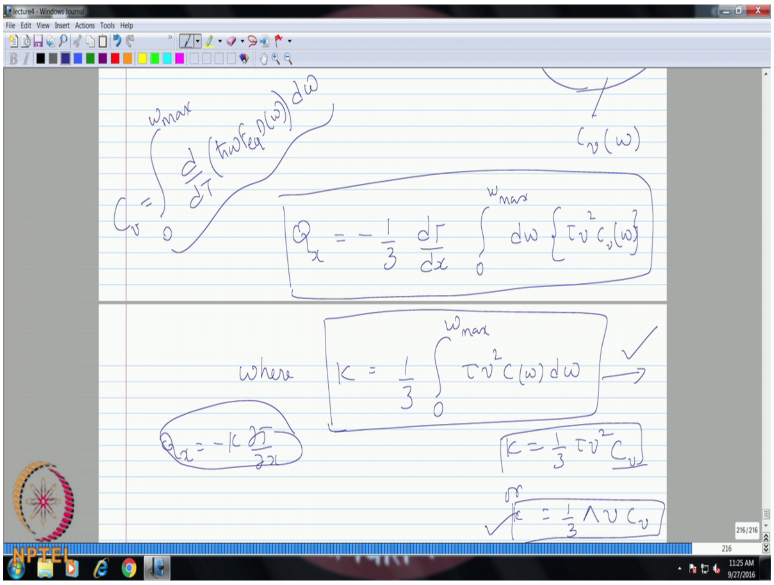

Student: (Refer Time: 18:23).

1 by 3.

Student: (Refer Time: 18:27).

0 to 2, Omega max you have tau v square c of omega d omega if you express this integral with the quantity called thermal conductivity then this becomes your Fourier's law. Therefore, now you get your minus k dt by dx. So, in this case we introduce quantity called thermal conductivity. Now which is basically related to your relaxation time your phonon velocity and your specific heat capacity for a given micro state if your tau and v are assumed to be constant independent of omega. So, then this can be simply taken out and this can be written as 1 by 3 tau v square c v that is it, or in terms of mean free path.

Student: (Refer Time: 19:40).

How can we write in terms of mean free path 1 by 3?

Student: (Refer Time: 19:56).

Now, go back to your kinetic theory expression what we derived from kinetic theory which we called as an approximate way of deriving and you compare this expression with that. So, what do you find from a kinetic theory same correct. So, there; however, the more accurate expression is, what this one a kinetic theory they cannot basically predict this, it only predicts this that is case where your relaxation times are frequency independent.

But never the less it gives a very good order of magnitude prediction. So, we derived the same expression from kinetic theory. So, we considered one interface we considered the flux of the phonons travelling in the positive x flux of phonons travelling in the negative x. Therefore, net flux and from that we have determined the expression for conductivity which turns out to be the same as a frequency independent case. Therefore, the more rigorous expression would have been this one. So, we have now, therefore, shown that what we call as Fourier's equation although people call this as constitutive relation and hypothesis in the macro scale you should understand that they are not really hypothesis, but can be derived from the sub continuum equations. So, in the in the sub continuum we do not have to define a property like conductivity.

So, it is all function of the phonon velocity relaxation time heat capacity and so on. But we can relate all these to the thermo physical property called conductivity and therefore, we can say that this is your Fourier's law correct. So, the same this is a very useful way of deducing many constitutive relations. So, not only the Fourier's law, but we can also do this for example, to deduce ohms law. So, may be to just give you another example. So, let me do this also for the charge flux similar to the heat flux here. So, the electron charges flux.

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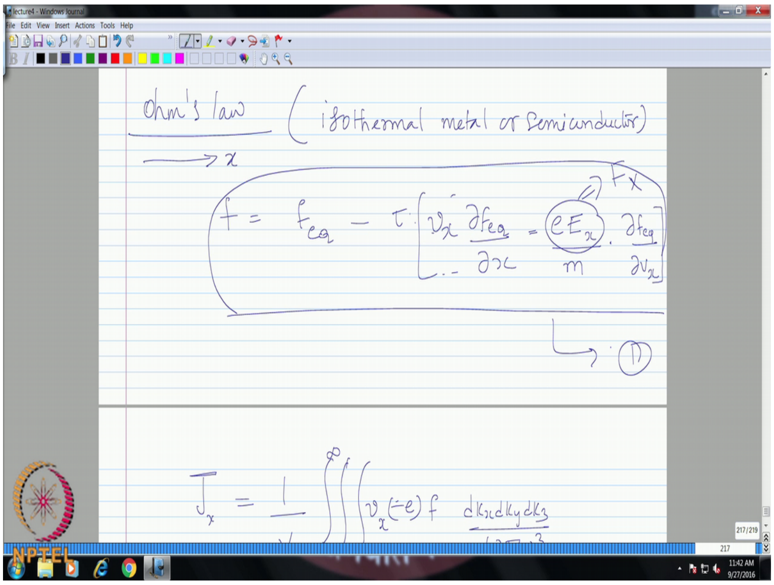

So, we will also now use this to derive the ohms law you can also use this to derive the Newton's law of viscosity where in the case of molecules. So, there the f equilibrium will take the form of the Maxwell Boltzmann Distribution which is the continuous distribution. So, you do not have to do a summation there everything is a continuous integral. So, all these conversion from summation to continuous space and then converting that to density of states all those things are not required.

So, it becomes much simpler to directly deal with the Maxwell Boltzmann Distribution, but let us look at the case of ohms law. So, probably you can start with the basic steps are similar. So, the way we are going to find the flux except that instead of heat flux we will have the current flux and therefore, instead of h bar omega. So, we will have the charge of an electron minus e the rest of the procedure is similar you have to multiply the non equilibrium distribution function to the corresponding charge corresponding velocity that is the charge flux which is your current flux.

Therefore, similarly you will you will be doing the same conversion you can do that again from the summation to continuous integral and use that density of states except now you are dealing with electrons. So, instead of omega you will have d as a function of energy e for density of states for electrons should be used and again, when you substitute for f in terms of f equilibrium. Now when you have a charge flux or current you have associated electric field. Therefore, this term will not be 0 correct. So, you have a electric field you have a corresponding force now that force is called the Lorentz force. So, that is due to the electric field and the flow of electrons. So, the electrostatic origin is the Coulomb force the electrodynamics flow is the Lorentz force. So, you substitute f in terms of, how do you relate your electric field?

Student: (Refer Time: 25:47).

F minus e Q is the charge which is minus e times capital e capital e is the electric field. So, this will give you the Lorentz force. So, just substitute that and you therefore, come to the expression till somewhere here. So, you will have an expression in terms of density of states and then substitute for f in terms of f equilibrium. Can you all attempt that? So, exactly the same similar system, but instead of flow of phonons we have flow of electrons and they are transporting charge not heat, now in a real conductor the electrons will semiconductor or metal can do both it will it will transport charge flux as well as heat. So, from the generic thing we will make an approximation specific approximation here if you are considering only charge transport the other things and then, but till that point can you all start.

Therefore, to derive the ohms law you can assume that the entire metal or semiconductor material is isothermal there are no temperature gradients the temperature gradients comes in then again you have simultaneously transport also along with charge transport. Therefore, to derive the ohms law you can assume isothermal metal or semiconductor. Therefore, how do you write the relation between f and f equilibrium first step the f will be equal to f equilibrium minus tau into?

Student: v x.

V x and then you have let me go step by step. So, I have tau and the first term is v x times b f equilibrium we have the charge transport only in the x direction will assume. Therefore, b f equilibrium by dx, you do not have gradients in the other direction. So, these are very certain points now see the way we have done the phonon on transport. We have written these gradients in terms of d f equilibrium by dt into dt by dx because, we have a temperature gradient there f equilibrium is a function of temperature. So, it is related to x true temperature understand. So, f equilibrium is not direction function of x, but it is a function of temperature and temperature is the function x. Therefore, we have split this as d f equilibrium by dt into dt by dx. Now, when you say charge transport, there is also going to be gradient of what.

Yeah voltage, you have the Fermi level e f is going to be a function of x this Fermi level is now consisting of two things one is your that is your voltage gradient that is one thing that is the electro static thing rather is electro chemical potential. Therefore, combination of these 2 wills your Fermi energy level. So, when you say there is a gradient of concentration charge concentration as well as there is there could also be a flow of electrons due to gradient of the electro chemical potential. So, together; that means, now d f equilibrium will be a function of dx through your gradient of electro chemical potential which is related to your Fermi energy level e f.

Therefore, it can be express is d f equilibrium by d E f into d E f by dx. So, that is the first step. So, we write down as now d f equilibrium by dx, but we can split this into d f equilibrium by d E f into d f by dx what is the second term now we also have an electric field or the Lorentz force term. We have minus e times the electric field magnitude in x direction e x by m and what is the corresponding derivative d f equilibrium by corresponding velocity in the x direction d v x.

So, this we can now write in terms of d E f and. So, on you will do that. So, this is your starting point. So, I am just expressing this f is equal to f equilibrium in terms of this right now, that is the first step. So, where this is your Lorentz force f x now can you write down the expression for the current flux we will use the notation j for current flux in terms of Q for heat flux.

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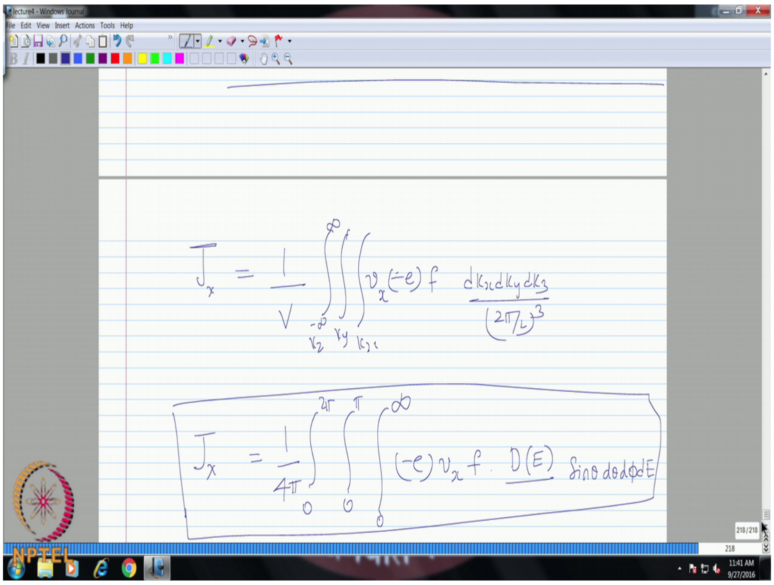

So, this will be equal to in terms of a write down in directly in terms integral; that means, you convert this summation into integral space for k. So, that is kx, ky, kz going from minus infinity to plus infinity. For example, what do you have for charge flux you have minus e you have v x you have f. So, this will give you the charge flux, if you divide it also by and you have dkx dky dkz divided by 2 pi by l whole cube, now this will give you the charge flux or current flux what is the unit of current flux.

Student: (Refer Time: 36:35).

Ampere per meter square, from this point, now we can use the density of states to convert all our integral from a case space to energy space because, we can always relate wave vector to energy through the density of states. So, do that conversion and what do we get and also you resolve this into a sphere and therefore, cause this in terms of polar angle and azimuth angle and energy. So, the three integrals kx ky kz gets converted into polar angle as azimuth angle and corresponding energy integral. I will use the substitute x to denote flux in the particular direction. Therefore, you have 0 to 2 pi 0 to pi and energy is 0 infinity minus e times v x times f times the new convert this through the density of states you have 1 by 4 pi, you have sin theta d theta d psi d E please check this it should be able to get to this point if you are able to comfortable to get this point; that means, you can your understanding what do you are doing.

So, we are defining the density of states similar phonon density of states except the density of d of omega we have d as a function of energy your e e. Therefore, similar to this we have instead of h bar omega we have minus e v x f we have sin theta d theta d phi d of e d E we should get a similar analogue expression is a clear everybody is able to reach this point right any questions on this. Now, you can go ahead and substitute the expression for f. So, before we substitute just let me call this as one let us now express this in terms of the right functions.

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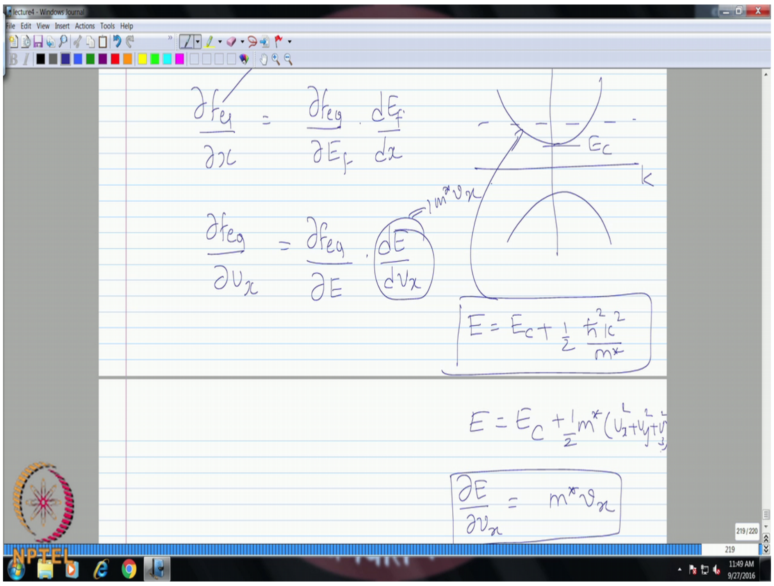

For example; as I said d E f equilibrium by dx can be expressed as d f equilibrium, now f equilibrium is a function of x only through the Fermi energy level because this is what the Fermi derive distributed function. For electrons and in Fermi Direct Distribution Function f equilibrium is a function of e, e equilibrium and temperature and when, you say gradient. So, your equilibrium distribution function now can be a function of x only through the gradient of the Fermi level e f.

Therefore, this is d equilibrium by d f into d E f by dx at there be in a temperature gradient and no charge flux transport this, will this would have become d E f equilibrium by dt into dt by dx and there will be a no electric field. So, then you will be able to get an analogues expression for transport of heat by electrons similar to that of the phonons except that the relaxation time will be relaxation time for electron-electron collision not phonon-phonon collision that is the only difference understand. So, this is how we also did this in the kinetic theory you can consider whether these are gas molecules or these are phonon gas or these are electron gas we get similar expression you have to only use the corresponding values velocity of that energy carrier relaxation time similarly with the heat transport from the Boltzmann equation.

However, when you are considering charge transport you can isolate it separate from heat transport and say this is isothermal and derive the charge transport because charge transport by itself is quite complicated. Now you can also have a case where charge transport is happening along with heat transport thermo electric effects Seebeck effect and Peltier effect, if you heard about them. So, you apply temperature gradient and there is a flow of current.

So, there is a coupling of temperature gradient and charge transport. So, in that case it becomes a more complex function we can also derive from the Boltzmann equation all the thermo electric effects including what is the expression for Seebeck coefficient and so on. In a very simple fashion, but a again there f equilibrium will also be a function temperature ok right now we are not assuming that temperature gradient is existing to simplify the case. Therefore, this is the relation similarly if you are looking at d f equilibrium by d v x, how is it a function of v x through which variable.

Student: (Refer Time: 42:50).

Hm.

Student: Mu (Refer Time: 00:53).

Mu is your Fermi level you can say that is a, your electro chemical potential mu at 0 Kelvin that is your Fermi level. So, that is function of x, when you have a charge gradient now what I am asking is what is the gradient in the velocity space, momentum space through which variable it is the function definitely not e f. So, what are the other remaining variables? Temperature definitely not then e e itself because remember the dispersion relation dispersion relation for electrons we made a parabolic approximation e verses k you remember. So, we have like this conduction band, valence band hopefully you remember that for metals the Fermi energy level is write inside the conduction band therefore, we have made an approximation as a parabola, and we have written the expression for e as therefore, e c we can say this is your starting of your conduction band plus half of h cut square k square.

2 m star. So, this is for the crystal. So, we called this as an effective mass of the crystal this is not the electron mass. So, because h cut square k square by 2 m comes from solving the equation if, you consider the free particle. But if you consider the entire crystal now we have the effective mass and star. So, this is your dispersion relation for this particular approximation parabolic approximation and we can always shuttle back and forth between k and v h h cut k is nothing, but m v momentum. So, the Boltzmann transport equation we can always rewrite this in terms of either k, gradient of k or gradient of v we can always shuttle back and forth.

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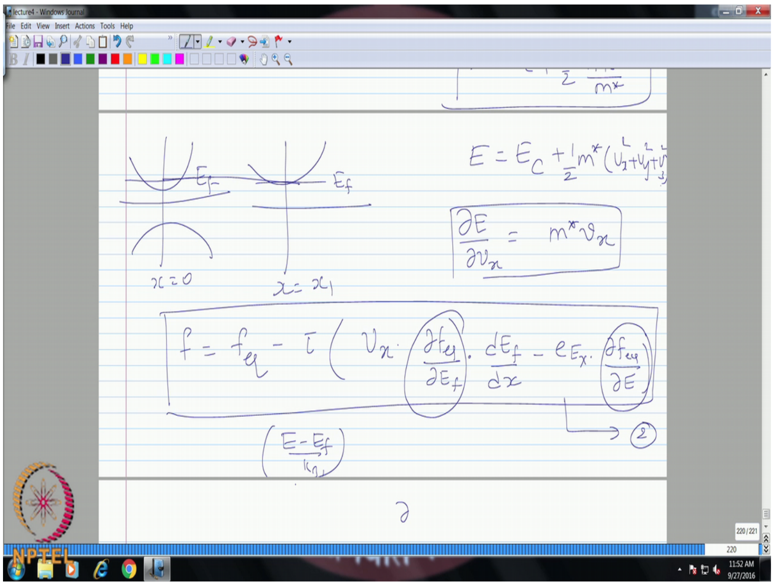

Therefore, we can simply express this as plus half of m star into v x square plus v y square plus v z square is that.

Therefore, when you say now de by dv x.

Therefore, what will be the expression m star v x.?

Student: v x.

So, when you therefore, say d v equilibrium by d v x so, it is a function of v x through d E right into d E by d v x and this is what m star v x. Now, you can substitute this into f therefore, this will become f equilibrium minus tau you have v x times d v equilibrium by d E f into d E f by dx this is a first term second term will be you have a minus e E x into. So, there will be one over m and m star this two will cancel of. So, you have d f equilibrium by d e. So, there will be. So, this m is actually m star for this case this is effective mass. So, that cancels of. Therefore, you have let us call this as equation number 2 yes.

Student: (Refer Time: 47:41) actually particular for a (Refer Time: 47:44).

Which one?

Student: Like Fermi level of (Refer Time: 47:48), so will be very.

So, that will be fixed if you consider only equilibrium if you have a non equilibrium. So, you are looking at different states now you are having along x.

Student: yeah along x.

Different values of Fermi energy then only there can be a transport of gradient to transport the electrons.

Student: (Refer Time: 48:18).

You understand. So, when you are talking about if you want to draw this now a different x. So, I will draw e f at x equal to 0 and then I will draw somewhere e f, somewhere here. So, there is a gradient at this is that x equal to x 1. So, this gradient is the reason why electrons are moving from x equal to 0 to x 1 in non equilibrium case. Therefore, e f is not constant it is now a function of x right. Now, the remaining part is therefore, to relate d f equilibrium by d E f to d f equilibrium by d E how is the related. So, you right down the Fermi direct distribution function take the derivative with respect to e f take the derivative with respect to e. So, you have exponential of v minus e f by k b t. So, how will they be related?

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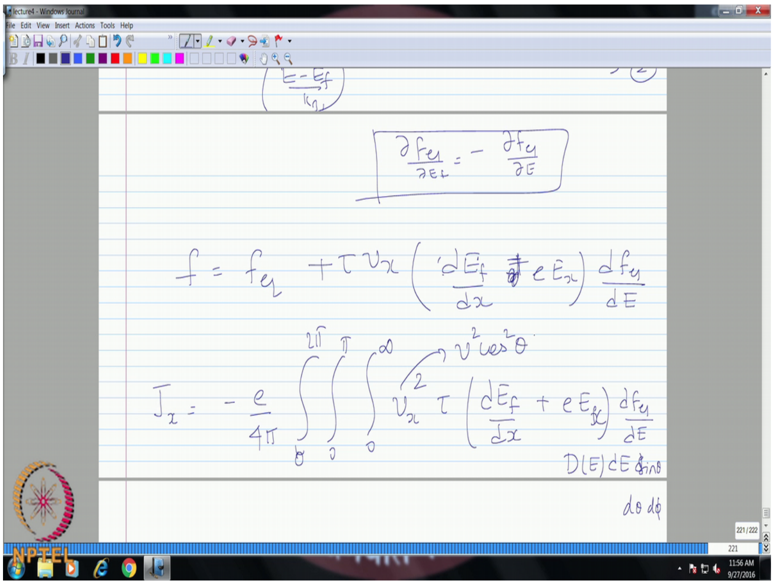

So, they are say you can say f equilibrium by d f will be equal to minus d f equilibrium by d E that is it correct. So, you have a plus e you have a minus e f. Therefore, you can also take derivative and check so, but without wasting much time will directly use this in substitute for f you will be able to get f equilibrium plus tau v x into dx equilibrium by sorry make sure making any mistakes here, this is d f by dx plus e E x I think some sign is a problem here and I am taking d f equilibrium by d E.

So, this is minus correct, but this should be a minus here right. So, this is d f equilibrium by d E. So, this should be a minus please check that ha no that is that is fine. So, minus of minus is plus right. So, I take one minus sign out therefore, this becomes plus and minus of minus is plus. So, is this clear? So, what I am writing is d f equilibrium by d E f I am writing this is minus d f equilibrium by d and substituting there and taking that common taking that common factor out. So, if I substitute this into therefore, the expression here for the current flux. So, that will be the final step. So, I write down therefore, j x I can write this as minus e by 4 pi. So, I can do this integral 0 to 2 pi 0 to pi 0 to infinity and then I will have a v x square tau and I also use the fact that integral over the solid angle f e equilibrium will be 0. Therefore, only the second term will be here I have d E f by dx plus e E x times d f equilibrium by d E into density of states d E d e d sin theta d theta sin theta d theta d phi.

Now vx will be nothing, but v into v square. Therefore, cos square theta now again integral cos square theta integral 0 to pi cos square theta into sin theta d theta is nothing, but 2 by 3.

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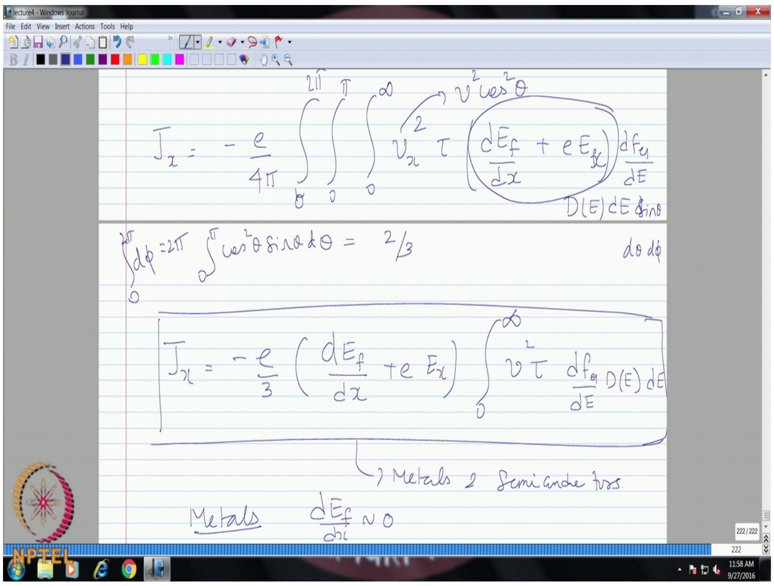

You can substitute that and therefore, and also the fact that integral 0 to 2 pi d pi is equal to 2 pi therefore, you will be getting minus e by 3 times, now all these are not functions of e. So, you can take this as outside d E integral over e plus e E x and you have 0 infinity times v square tau d f equilibrium by d E d of e into d E right. So, finally, we have reached the point to this is the final step.

Now this expression is common to both metals and semi conductors. So, for the case of metals when you are applying only this to metals we can assume that since you have. So, many number of free electrons the number density of free electrons are too many you can make an assumption that the change in the Fermi energy level is not that much the gradient. So, we can put this to 0 because, the number density is already too large to therefore, you may have some change, but it is not very significant because of the large values of electron number density. Therefore, you can put this approximation for metals.

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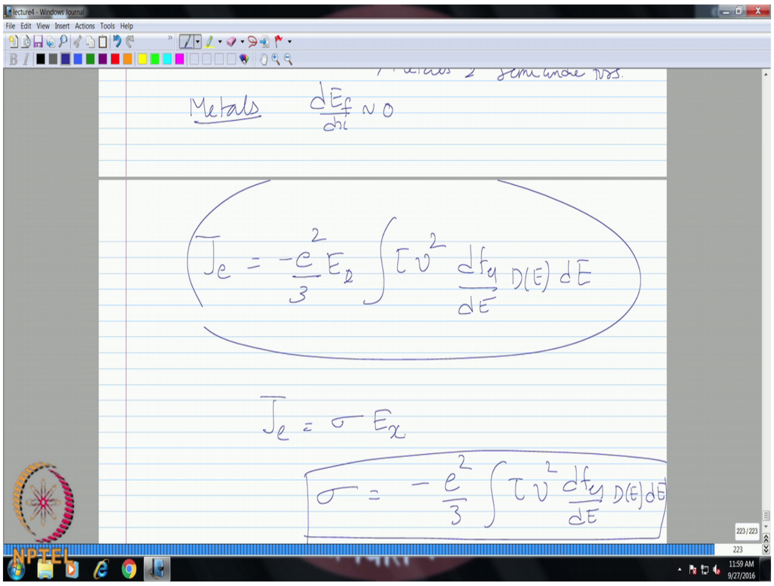

And therefore, what do you gets for metal is minus e square by three e x tau v square d f equilibrium by d E d of E d E. So, this is your ohms law provided you recognize that the way you write your ohm's law is currant flux is equal to electrical conductivity times the electric field. So; that means, your sigma should be equal to minus e square by three integral tau v square d f equilibrium by d, d of E d E. So, this will be your expression for electrical conductivity.

So, we will make one more approximation into this to make it much simpler and tomorrow will complete that exercise. So, basically this is your ohm's law I mean except the facts if you want to write it in terms of electrical conductivity we have the expression for electrical conductivity similar to the thermal conductivity we write this as function of the relaxation time of electrons velocity and so on. In similar manner you can also derive the expression for thermal conductivity of electrons. So, there you do not have any electric field you have only temperature gradient. So, tomorrow we will make the next step here and then will conclude this portion and then, we will move on to doing some problems which involve the transport process in a small film nano scale film perpendicular to the film. So, these real time problems we will try solve 1 or 2 of them.

Thank you.