Micro and Nanoscale Energy Transport
Dr. Arvind Pattamatta
Department of Mechanical Engineering
Indian Institute of Technology, Madras

Lecture - 23
Boltzmann Transport Equation under the Relaxation Time Approximation

Good morning, today we will look into the details of Boltzmann transport equation, yesterday we derived I mean derived in the sense that it is not a very rigorous derivation, but we showed that for a one particle distribution. So, you basically convert the complex linear equation into a kind of solvable form of the Boltzmann transport equation. So, this is the more practical equation to solve concerning the practical distribution compared to the more complex computationally expensive linear equation; however, you end up with having an additional term the Boltzmann equation which is the collision term. So, you have to somehow learn to deal with the complex city involving collision and coalition is actually in physics this a multi body problem; that means, many body problem involving the scattering between at least minimum of 2 particles and it can also be extended to large number of particles, even for a 2 particle system, if u want to express the coalition term this written as what we call as the scattering integral.

From present state which is u know say K is your present state is your wave vector and it collides with another particle which is having K 1 is the wave vector of other particle and the after collision the respective wave vectors becomes K prime and K 1 prime. So, we want to therefore, integrate this over the other wave vectors values for K 1, K prime and K 1 prime and therefore, we are calculating what is the net change in the wave vector due to scattering from its present state to another state for example, from say K to K prime and the other one is the scattering which is coming from scattering from another state which is probably K prime and if it scatters it wave vector come back to state K. So, the net change in this out scattering minus in scattering will be v scattering integral. So, which has to be integrated over the all other wave vectors space except the current wave vector which is K.

So, therefore, this gives u the scattering integral and just the collision rate of change of distribution due to collision. So, this is a very complex integral to evaluate and again therefore, people maybe in physics have tried for some simply system, but not very useful therefore, what people do is they apply what is called as the relaxation time approximation.

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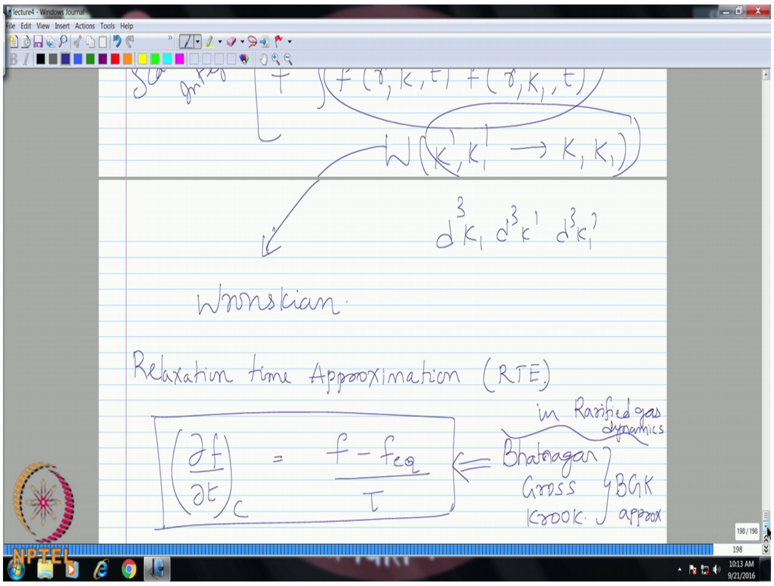

$\int f(\gamma, k, t)\, f(\gamma, k_1, t)$

$W(k', k_1' \to k, k_1)$

$d^3k_1\, d^3k'\, d^3k_1'$

Wronskian.

Relaxation time Approximation (RTE)

$$\boxed{\left(\frac{\partial f}{\partial t}\right)_c = \frac{f - f_{eq}}{\tau}} \Longleftarrow \left.\begin{matrix}\text{Bhatnagar}\\ \text{Gross}\\ \text{Krook.}\end{matrix}\right\} \text{BGK approx}$$

in Rarified gas dynamics

So, this it is a very simplistic, but very a practically useful approximation. So, what they say is that the you are entire scattering or collision term that we have on the right hand side can be simply expressed as a change from the equilibrium function. So, we can write this as f minus f equilibrium divided by some time scale tau. So, In fact, it should be I think the way we have written it yes, this is fine this is your simplest way of dealing with the collusion now you will see that in this picture there is nothing we talking about 2 particle interaction and how the wave vector changes after collision and all that there is no information of any of this particle approximation.

So, the inspiration for this comes from using what we call as the Bhatnagar gross Krook approximation Bhatnagar gross Krook. So, this is simplified as b g k approximation this is quite common in clarified gas dynamic. So, in the clarified gas dynamic is also the Boltzmann transportation equation is also used and there is also a similar problem with collision between the gas molecules and there we bring in b g k approximation very similar to the 1 that we have written here. So, we take an analogy from the gas molecule theory or gas kinetics and then we apply that to also the other energy carriers and simplify the collision term. So, you should understand that this is a huge level of simplification starting from where we, where we looked into the complex coalition integrals and so on. So, we have drastically simplified the collision integral with something which is quite different, it does not describe anything about the change in the wave vector space and all that, but what this physically signifies is that if you put this back into the Boltzmann equation. So, for example, we have written the Boltzmann equation here, if you substitute in place of right hand side and you ignore all your advection terms that is the rate of change of position and in the case there is no external course there is no change in the momentum also.

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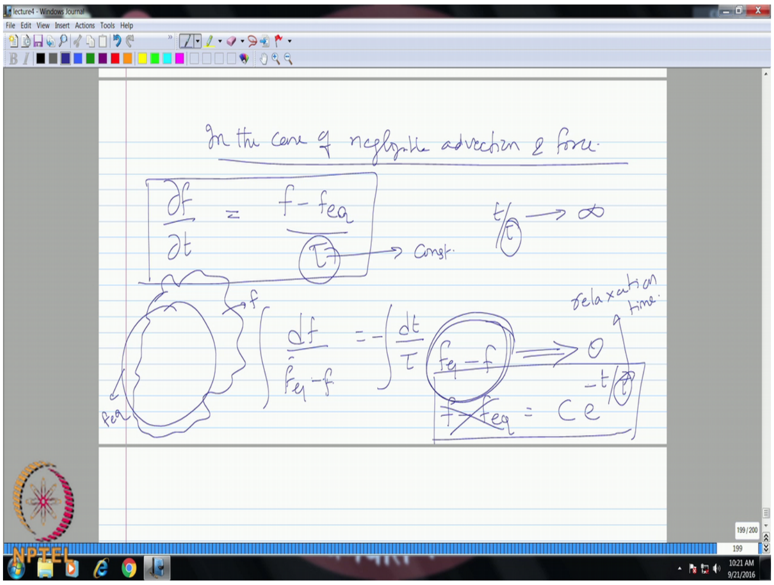

In the case of negligible advection & force.

$$\boxed{\frac{\partial f}{\partial t} = \frac{f-f_{eq}}{\boxed{\tau}}} \longrightarrow \text{Const.}$$

$$t/\tau \longrightarrow \infty$$

$$\int \frac{df}{f_{eq}-f} = -\int \frac{dt}{\tau}$$

$$\boxed{f_{eq}-f} \Longrightarrow 0$$

$$\boxed{\cancel{f-f_{eq}} = C e^{-t/\tau}}$$

relaxation time.

So, in that case you have the time rate of change of distribution function on the left hand side on the right hand side you have the b g k approximation. So, in their case of negligible advection and force therefore, we can find out the solution for this for the simplest case there is no change in momentum space there is no change in the physical coordinate the distribution function only changes with time right, this is a simplest possible solution that you can think of what happens. So, what do you get here you have d f by f minus f equilibrium is equal to d t by tau to find out integrated find the solution I will come to the physical explanation of tau. So, through this we will able to interpret what exactly tau is yes you can assume right now it is a constant. So, u can assume that your tau is a constant this has units of time, but it is different from the actual physical time yes. So, we have f minus f equilibrium is equal to c e raised to t upon tau. So, this is the solution for this case where distribution function is not a function of space and momentum, but it is only function of time. So, from this you can get a feeling of what this tau or relaxation time this is called the relaxation time now right what does tau signify here. So, if you are looking at t by tau which is quite large going to infinity it should be e power minus, I think we have made c power I think it should be f equilibrium minus I think we have to make this as f equilibrium minus f. So, that we know what we are talking about here just let me change this to f equilibrium minus f. So, will have a minus sign here therefore, this will be f equilibrium minus f and we have a minus sign.

So, what that signifies is large values of time going to infinity. So, what does it mean this is going to 0 so; that means, your non equilibrium function is approaching equilibrium distribution. So, you can imagine if you want to plot the equilibrium distribution this is the kind of uniform distribution in space. So, if you are supposed plotting this with respect to space or momentum space or physical coordinate space this is may be like a circle it is uniform it is not changing with any direction now, if you look at the non equilibrium function that will be now distorted like something like this. So, this is you say f equilibrium. So, this is your f. So, you are all the time looking at their difference between these 2 distribution functions and what it says is this relaxation time is some kind of time scale over which you bring the non equilibrium distribution function and you relax it to equilibrium distribution function.

So, this is a kind of time scale therefore, relaxation time indicates some kind of a time scale about which this relaxation of non equilibrium can take place. So, physical significance of the relaxation time is basically how long does it take for a disturbed system or system this which is actually having a non equilibrium in transport case to bring back this system to an equilibrium case. So, how does this bring back to equilibrium only through scattering only through collision right? So, this is how the collision is incorporated. So, entire collision is incorporated only through the scattering time or the relaxation time otherwise people may wonder what this to do with coalition is, but the information about the collision is completely buried into this definition of the relaxation time.

So, this tells you that through multiple collisions. So, the higher is a coalition rate the higher is a scattering rate the faster is the return to the equilibrium. So, or in other words if you are talking about smaller relaxation times what does it mean? Higher will be the collision rate; that means, the particles are probably packed, but close to each other. So, the relaxation times are smaller. So, quicker will be the return of the non equilibrium to equilibrium distribution function. So, this is the way that the Boltzmann transport equation with the relaxation time of approximation is used. So, now, the only unknown parameter that we have to find is basically what is this relaxation time and what does it incorporate and how do we calculate it. So, once you know that we can attempt to solve the Boltzmann transport equation.

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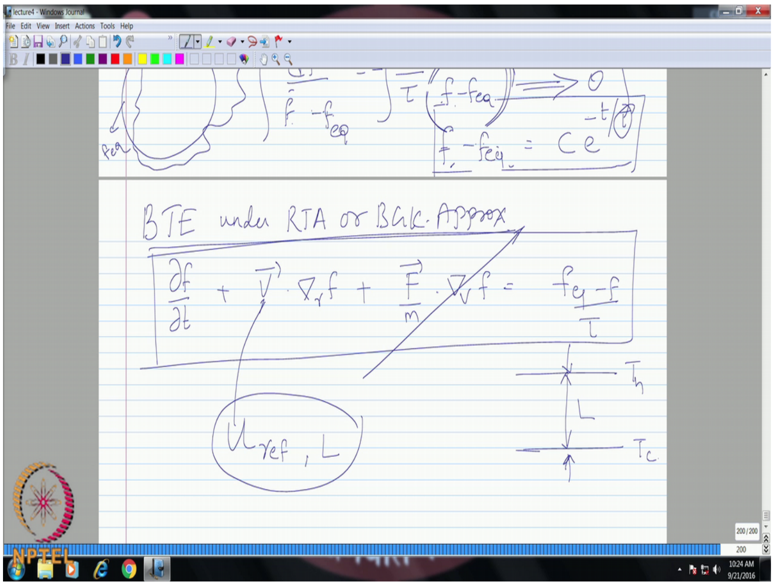

So, this is the very useful practical approximation that is commonly used to solve the transport problems. So, if once you substitute this into the d t. Now, therefore, you write. Let me check the signs if I am saying it is f equilibrium minus f it should be f equilibrium minus f right. So, yes it should be f equilibrium I think here, I should change the sign please correct it. So, this should be f equilibrium minus f here. So, therefore, this part again now changes to f minus f equilibrium, some correction regarding the sign this should be f equilibrium f minus f equal, here also f equilibrium minus f right? So, therefore, this is you are what we call as the Boltzmann transport equation in the relaxation time approximation. So, we write b g b t e under relaxation time approximation or sometimes people call this b g k approximation and what is. So, important about this Boltzmann transport equation now if you want to non dimensionalize this.

So, let us consider a case without any external force. So, let us for the time being ignore the 3rd term you can choose some reference velocity u reference for the sake of non dimensionalization right and therefore, you can substitute this reference velocity into the actual dimensional velocity, similarly you can choose a reference length scale for example, if you are talking about something like heat transport between 2 plates. So, plate on1e maintained at a higher temperature t h and plate 2 maintained at lower temperature t c. So, you are talking about the scale length scale which is the separation distance between the 2 plates which could be capital L.

So, therefore, you can use the length scale to non-dimensionalize as L this is your characteristic length scale. So, now, substitute the reference velocity and characteristic length scale try to get a non dimensional form of the Boltzmann equation. So, for the time being we have neglected the third term which is in the momentum space we do not want to non dimensionalize that now and see what happens you do not have to non dimensionalize the distribution function distribution function anyway just a number density you do not have to non dimension only non dimensionalize the time velocity and position.

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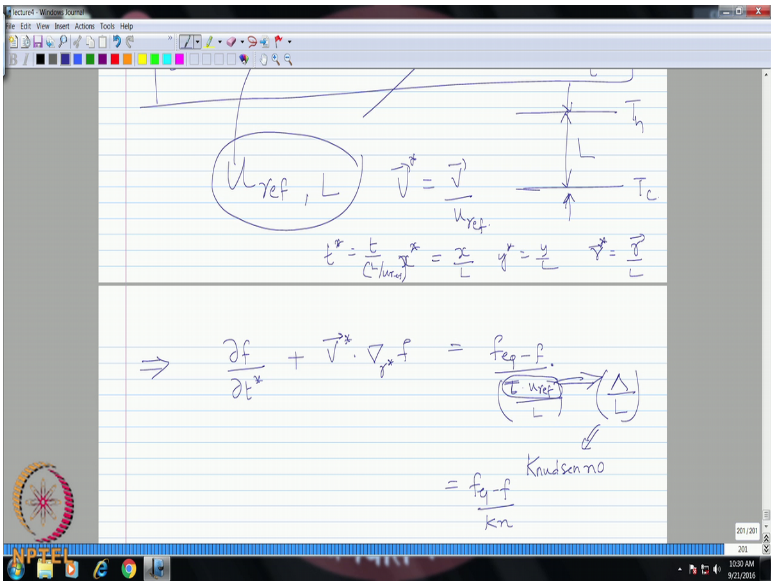

$$\boxed{u_{ref}\,,\ L} \qquad \vec{v}^* = \frac{\vec{v}}{u_{ref}}$$

$$t^* = \frac{t}{(L/u_{ref})} \quad x^* = \frac{x}{L} \quad y^* = \frac{y}{L} \quad \vec{r}^* = \frac{\vec{r}}{L}$$

$$\Rightarrow \frac{\partial f}{\partial t^*} + \vec{v}^* \cdot \nabla_{r^*} f = \frac{f_{eq} - f}{\left(\frac{\boxed{\tau\, u_{ref}}}{L}\right)} \rightarrow \left(\frac{\lambda}{L}\right)$$

Knudsen no

$$= \frac{f_{eq} - f}{Kn}$$

So, you can call something like v star is equal to v vector by u reference and something like x star or r star whatever you want to call x by L y star as y by L or whatever, or you can say generally r star is equal to r vector by L. And you can call t star t by some other scale now, in this case what will be the time scale now based on the reference velocity and characteristic length L by u ref. So, you have d f by final non dimensional form d t star plus v start r star let us say f, on the right hand side we have f equilibrium minus f by tau. So, what else will be there? So, we have a u ref u ref by L. So, this should be L by u reference upon n right.

So, therefore, now we can define. So, this is tau into u reference, how do you define? What is the definition of; what is the relation between relaxation time and mean free path? This is your mean free path right? So, therefore, this is your mean free path divided by L. So, what is this is your Knudsen number. So, therefore, the non dimensional form of the d t will have on the right hand side the corresponding non dimensional number which is your Knudsen number. So, this is just like your non dimensionalizing your fluid mechanics or heat transfer equation. So, there you will have Reynolds number fantle number similarly here you have the characteristic non dimensional number which is your Knudsen number. So, that is what it says if you are talking about continuum that is the case where the Knudsen number what is the limit for continuum going to 0.

So, what does this tell about this equation when the Knudsen number is going to 0 what happens to the equation now look at the terms.

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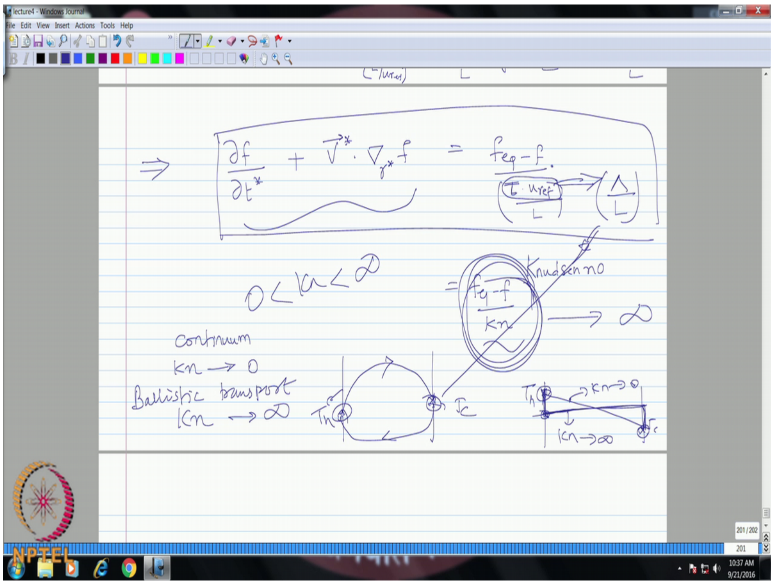

So, this term will now go to infinity. So, this will become the significant term right therefore, this scattering will become the most important term for the limiting case where you are approaching continuum that is because you have now too many energy carriers. So, they can collide.

So, advection process will be very insignificant compared to your coalition process. So, then that is your diffusion limit. So, all your macroscopic loss of continuum can be derived under this particular condition. So, for example, fouriers equation right Newtons shear stress loss for ohm's law flicks law of diffusion all this can be derived under the limits where you have you are dominated by diffusion, diffusion is nothing, but coalition of the energy carriers. So, this is possible only you are talking about very small Knudsen numbers where the scattering term becomes varies very significant and more dominant compared to the advection term.

On the other hand if you are talking about high Knudsen numbers Knudsen number is going to infinity. So, this is you are what is this limit free molecular limit if you talk about gas dynamics, if we talk about nanoscale generally this is called ballistic transport; that means, in this case what happens to this term 0. So, there is no collision at all right. So, Knudsen number is infinity there is no collision between the energy carriers; that means, the transport is ballistic it is like a missile, if you talk about a high temperature body and low temperature body here. So, the energy carrier from here directly goes hits this particular boundary right. Similarly energy carriers at this temperature will directly fly and hit this particular bond in between there are no energy carriers to collide and transfer the information.

So, this is called a ballistic limit. So, they are just directly like a project time shoot at shoot shooting from 1 boundary to the other and therefore, what happens there will be a shock. So, when this energy carrier sees flies to the 2nd boundary it will encounter a different temperature right. So, this has an equal for example, this has certain distribution based on the temperature of this odd surface and now it goes and encounters the 2nd surface which is at a lower temperature, but it does not know that information because there are no energy carriers in between. So, there will be a shock. So, if you solve this particular problem using the Boltzmann transport equation. So, what do you expect is suppose this is your T h and this is your T c, there will be a temperature jump like this and something like this and again a temperature drop like this. So, the phonons if you are looking at solid the phonons cannot transfer basically all this information to the cold side and similarly the cold side information is not transferred to the hot side.

So, the phonons will have an energy density which is somewhere in between these 2 temperatures at the boundaries there will be a discontinuity. Because the phonon which is coming from the cold side will have a lower density compared to the boundary similarly the phonon going to from the heart to the cold side will have a higher energy density compared to the cold bond therefore, it has to only now have a discontinuity as a solution as and when you are Knudsen number keeps smaller and smaller you are approaching the continuum limit. So, you find finally, for Knudsen number going to 0 what will be the solution how will the solution look? This is your linear based on you are fourier equation linear profile this is you are classical conduction profile right and why this conduction profile is linear because it is dominated by diffusion.

So, when you do not have any information propagation by diffusion it is completely only advection which transports and therefore, you have this. So, this profile will be for Knudsen number of infinity and this is your diffusion limit. So, now, you understand that the Boltzmann transport equation is a self sufficient equation it carries all the information regarding what kind of regime you are working with. So, you do not have to worry whether you have to solve separate equation at Knudsen number going to 0, because the same equation Boltzmann transport equation will be equivalent to the continuum equations at that limit whereas, it will also behave like a proper nanoscale transport equation at larger Knudsen numbers. So, therefore, this particular equation here is valid for all the Knudsen number ranges from 0 to infinity right. Because it can recover the continuum equations on the lower Knudsen number regime on the higher Knudsen number regime it will become a unique solution. So, let us understand therefore, little bit how to calculate these relaxation time and what does it basically involve right. Now, when you are talking about scattering?

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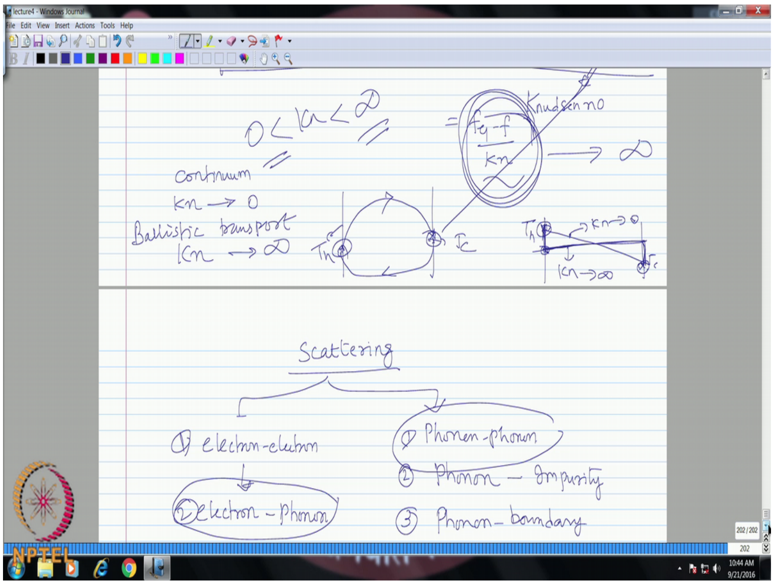

So, this is a very important topic because the relaxation time is now as I said all the information about the coalition and scattering between the energy carriers are buried into this particular parameter. So, therefore, what are all the different modes of scattering and how this information has to be conveyed to tau?

So, 1 of the important modes of scattering is if you take the case of electrons it is electron scattering for example, if you take the case of phonon you talk about phonon scattering similarly for gas molecules. Now, if you are looking at solids for example, semiconductor their phonon transport is the most dominant. So, it is not only phonon scattering, but you also have phonon scattering with other things such as impurities if you are doping the semiconductor make it either p type or n type. So, this are external impurities and. So, these impurities are dislocations in the crystal will cause a resistance to the flow of this lattice vibration. So, when you model these as particles again you have to think about scattering of phonons with these dislocations or impurities. So, therefore, you can have a 2nd type of scattering which is your phonon impurity scattering because the impurities themselves are not a physical carrier.

So, they are some kind of resistance to the flow of phonon and the phonons have to encounter them most likely they cannot pass through these impurities. So, they get scattered and that is a certain scattering time associated with that and finally, if you are talking about the high Knudsen number cases what happens to the phonon? Which is traveling from the left to right, assume that is no impurity here there are no other phonon. So, there is no phonon scattering there is no phonon impurity scattering. So, we can say that the right hand side term goes to 0, but you also have a phonon boundary scattering the phonon just does not go and get stuck to the boundary it also gets scattered from the boundary surface.

So, it is a physical boundary and the phonons cannot propagate through them. So, therefore, the 3rd kind of scattering is a phonon boundary scatter, similarly for the electrons you can also talk about all these and you also have in most of the metals and semiconductors electron phonon scattering very important. Because the electrons basically are free electron which can move about in the crystal and already you have this phonons. So, there are many instances where the electrons have to now collide with the phonons so. In fact, this is the reason why you have electrical resistance in the 1st place if there was no electron phonon coalition your resistance will be 0 the electrons can freely flow through the metals or semiconductor, but they are resisted by the phonon. So, therefore, you have a finite value of electrical resistance.

So, in order to understand physically things like electrical resistance thermal resistance you have to look at the individual scattering for example, electrical resistance can be explained by the electron phonon scattering and similarly the thermal resistance can be explained by means of phonon scattering. So, if you are looking at electron phonon scattering this is a highly inelastic scattering process. So, you have 2 different energy carriers colliding. So, your energy will change post collision your wave vector will change and also the coalition between electron and phonon will not be just like that. So, the electrons cannot interact with all kinds of phonons. The electrons will sometimes into it interact with the higher frequency phonons most likely the optical phonons and that will result in the release of some electromagnetic energy also.

All these possibilities are existing. In fact, they use many of these principles to make semiconductor based you know light emission phenomena and all this related to such kind of electron phonon interaction. So, let us particularly focus on phonon interaction because if you are looking at d transport in semiconductors. So, what happens is if you are talking about a system where you have 2 phonons.

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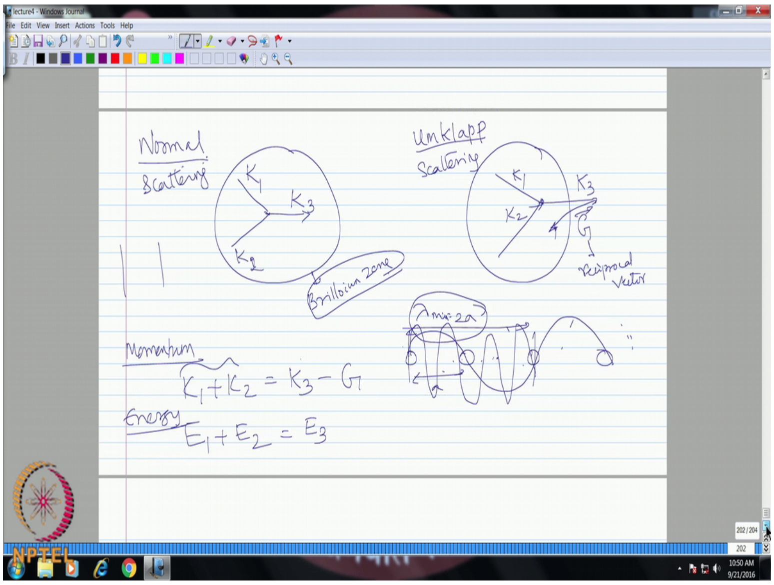

Momentum $K_1 + K_2 = K_3 - G$

Energy $E_1 + E_2 = E_3$

Let us say you have phonon 1 with wave vector k the other phonon wave vector K 1 and these 2 collide and you have a 3rd phonon which is formed these 2 common collide and then these are virtual particles. So, you can say after collision it be equivalent to formation of another phonon with a wave vector which is K prime. So, similarly if you are talking about let me use the standard nomenclature K 3. So, let me call yes, let me call this is K 1, K 2 and K3, let me not use this prime again because I have used this before let me. So, similarly you can have similar collision between 2 phonons K 1, K 2, but there is a difference between these 2. So, you can imagine this boundary what I have drawn is the boundary of the brillouin zone. So, this is the periodic repetition of this unit lattice structure and when we talk about the phonon minimum wave length. So, we talked about say monatomic lattice where we have this kind of a structure and what is the minimum allowable wave length.

So, therefore, if you are talking about this is you are a. So, therefore, this will be 2 times a. So, I have to redraw it not drawn its correct let me resolve. So, this is you are a here. So, therefore, the minimum allowable wave length will be 2 a. So, wavelength which is smaller than this does not make sense. So, you cannot have vibrations like this, which are much smaller than the lattice space. So, therefore, this lambda mean is equal to 2 a is going to define the boundary of the brillouin zone right. So, when we therefore, define collision between 2 phonons we have to make sure that the wave vector of the 3rd phonon is not greater than the allowable wave vector space within the brillouin zone. So, if this wave vector exceeds the brillouin zone wave vector. So, this will suppose to move out of the brillouin zone, but which is not possible because you cannot have vibrations which are smaller than the lattice spacing.

So, therefore, you have to correct this by pushing this back into the brillouin zone. So, you have to therefore, correct it by some reciprocal what we call as a reciprocal vector some correction is to be done. So, this is your reciprocal vector which makes sure that your solution is physical and therefore, we correct it by that much and we push it back into the brillouin zone. So, therefore, this kind of scattering where it does not exceed the brillouin zone space this is called normal scatter and the one which has to be corrected back using the reciprocal vector is called the unklapp scattering.

So, if you want to write the conservation of momentum and energy for the phonon scattering. So, in the case of the generic case for the conservation of momentum, we have K 1 plus K 2 is equal to K 3 for the normal scattering; however, for unklapp scattering minus g. So, this reciprocal vector will be 0 for the case of normal scattering, but is required for the case of unklapp, but whereas, we will talk about energy that is perfectly conserved. So, these are the pre collision values of wave vector and energy and this is the post collision value right.

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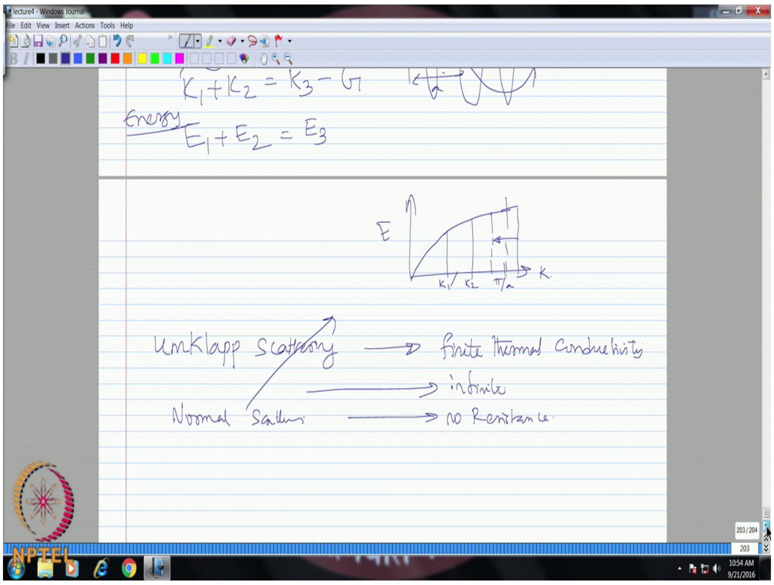

$K_1 + K_2 = K_3 - G$

Energy $E_1 + E_2 = E_3$

Unklapp Scattering → finite Thermal Conductivity

→ infinite

Normal Scatters → no Resistance.

So, in other words if you are representing by means of plot of E verses K for example, the edge of the brillouin zone is what phi by a. Therefore, if you are talking about the 2 phonons, one which is having k 1 the other which is K 2, K 1 plus K 2 if it is greater than phi by a. So, this is corrected by the reciprocal lattice vector and brought inside because this is your maximum allowable value of K, corresponding to the minimum wavelength lambda this marks the edge of the brillouin zone right so. In fact, if you take therefore, the normal scattering momentum is perfectly conserved and there is no problem.

Now in the unklapp scattering this is where the reciprocal lattice vector is used because now this poses a resistance now to the momentum, other words I mean in the normal scattering case there is no resistance to the collision of the phonons and transfer of momentum whereas, in the case of unklapp scattering there is a resistance to the momentum transfer. So, the momentum is brought down by means of this reciprocal lattice vector reciprocal. So, therefore, this is the one which results in the thermal resistance.

On a fundamental basis, if you want to describe why we have a finite thermal conductivity of a solid. So, that is because of the presence of unklapp scattering if there was no unklapp scattering your thermal conductivity would have been infinite because the phonons can flow easily without any resistance. They can transfer the momentum they can transfer the energy the conservation of momentum is satisfied. So, the momentum will not come down right so, but what is this resulting in the reduction of the momentum is the unklapp scattering which brings down the momentum and therefore, builds a resistance for the flow of heat.

So, this is the most important scattering mechanism when you want very when you are considering the effect of finite thermal conductivity. So, therefore, to summarize unklapp scattering process contributes to a finite thermal conductivity. So, if there was no unklapp scattering. So, you will be having infinite thermal conductivity and whereas, you are normal scattering does not contribute to any resistance no resistance. So, through this you therefore, you can explain through the electron phonon coalition you can explain the finite electric resistance and through phonon in unklapp scattering mode you can explain the finite thermal conductance. So, now, how do we therefore, calculate all these scattering modes we have normal scattering, we have unklapp scattering, we have phonon impurity scattering phonon boundary scattering.

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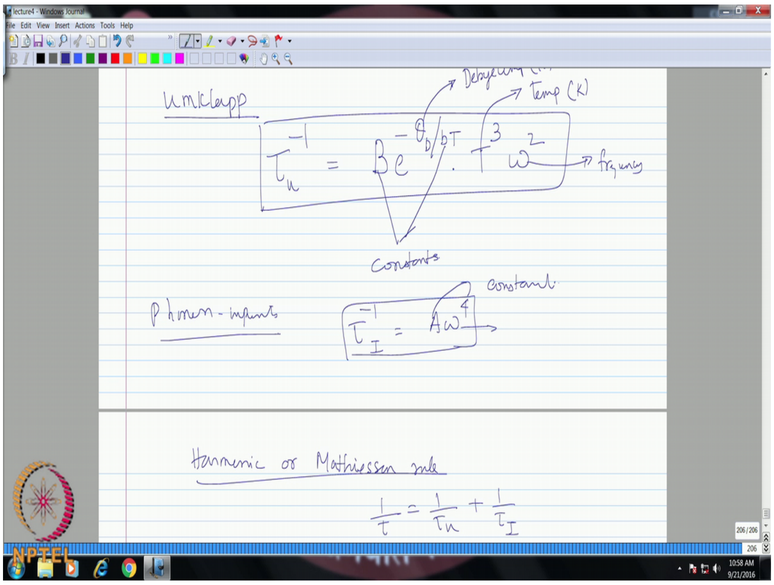

Umklapp

$$\boxed{\tau_u^{-1} = B e^{-\theta_D/bT} \cdot T^3 \omega^2}$$

Debye

Temp (K)

frequency

Constants

Phonon-impurity

$$\boxed{\tau_I^{-1} = A\omega^4}$$

constant

Harmonic or Mathiessen rule

$$\frac{1}{\tau} = \frac{1}{\tau_u} + \frac{1}{\tau_I}$$

So, how do we calculate all of this? So, there are some standards expressions which I would just like to give for example, if you take the case of unklapp scattering. So, the relaxation time has a particular empirical correlation this is like this. So, now, these are constant capital B and small b are constants and you are theta d you remember what it is you are d by temperature and t is you are actual temperature the physical temperature and omega is the frequency all this in Kelvin. So, depending on the kind of material these constants can take different values so.

So, this is how empirically the phonon scattering time is calculated, similarly if you are looking at phonon impurity scattering. So, the expression use this subscript is I a omega power 4, where is also another constant this phonon impurity scattering can be imagined like Rayleigh scattering in Rayleigh scattering also we have 4th power dependence to frequency scattering time that is the Romans scattering or whatever, we attribute the sky color is blue because the if you look at the frequency the higher the frequency the greater the probability of scattering. So, that is why we have this. So, this is similar to your Rayleigh scattering modes.

So, that is why we have 4th power dependence on frequency. So, therefore, we have all these different scattering relaxation times therefore, how do we calculate your total relaxation time. So, we use what is called as a harmonic mean or this is also called as Mathiessen rule which is just a harmonic average of therefore, 1 over tau will be 1 over tau u this is a unklapp scattering time and the other is your phonon impurity scattering. So, using the Mathiessen rule which is the harmonic mean of the different relaxation times you can get your final relaxation time and substitute into the b t. So, we will stop here.

Thank you.