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

Lecture - 24
Derivation of Continuum Laws from Boltzmann Transport Equation Part 1

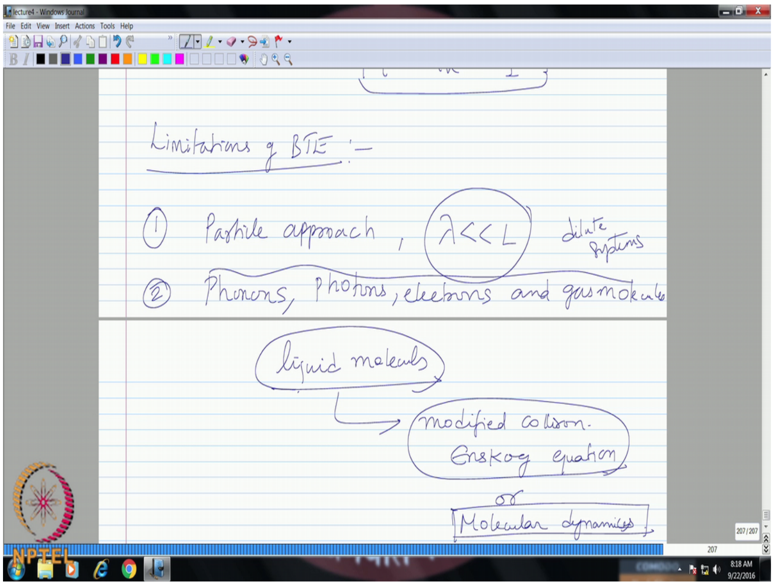
Good Morning. Yesterday we looked at the different scattering mechanisms when we solve the Boltzmann transport equation. These scattering mechanisms are necessary to calculate the relaxation times. We saw that for example, phonon scattering is very important, especially the Umklapp scattering; which gives the resistance to the momentum of the phonon transport and therefore, contributes to the thermal resistance and apart from that you can also think about other kinds of interactions or scattering between phonon and the dislocations or impurities in the crystal and you can also involve the boundary scattering of the phonons.

We have therefore different expressions for the relaxation times and the overall relaxation time that is used in the BTE can be evaluated using a simple harmonic mean or a matthiessen average. Once, I think you know the preliminaries of how to calculate the relaxation time, the next is to go ead and solve the Boltzmann transport equation and solution again depends on the kinds of problem that you are looking at as far as you are concerned about the recovery of the no Knudsen number regime, it is a continuum regime that can be done analytically.

So, this is what we will be doing in the next couple of classes, whereas, if you are looking at high Knudsen number regimes. So, that involves some rigorous solution we will see part of this part of you know the high notes and number transport, but the more detailed solution can be obtained only numerically which will be actually the computer assignment I was talking about. So, as far as within the classroom what we can do is, do some limiting cases especially the lower Knudsen number regimes are important because you should know that the Boltzmann transport equation can recover all the macro scale continuum you know constitutive relations.

This is what we want to show in the couple of classes, but before that, I want to also give you the limitations of this equation. So, this is not the, you know the unique equation which can give a solution to all kinds of nano scale problems, you have to know the limited range of applicability of the BTE and therefore, let us say, just let us highlight the limitations of the Boltzmann transport equation.

(Refer Slide Time: 03:23)



So, I mean one of the one most straight forward thing which you might already know is, that you know when we talk about BTE and distribution function and all these are limited to particle based approach that is if you are looking at another characteristic scale which is your wavelength. So, if you compare your wavelength with respect to the characteristic dimension. So, which is your probably the length of your thickness of your material. So, this should be much smaller than l in order for the particle approach to be valid.

If otherwise, then you end up with again considering the wave effects. Whatever we have studied in quantum mechanics pause considering the wave effects, but that was not clearly transport of heat for example. So now, what we mean is that we have to formulate a transport equation, which can study the wave nature and the corresponding transport of these waves. So, that is the electromagnetic equations the Maxwell's equations.

So, which deal with the transport of ways right? So, the approach now becomes quite different from what we have done so far. But we can safely say that most of the applications can be considered you know to have length scales which are larger than the wavelength and therefore, we can kind of ignore the wave effects in most of the cases.

Therefore, although we are limiting it to a particle approach, so in a wide range of applications, the Boltzmann transport equation is still used; that means, we are still looking at applications is satisfied this particular condition. And the other important thing is, what kind of energy carriers are I mean on what kind of media for which we can solve the Boltzmann transport equation. So, it can be used for a dilute system of particles such as, the phonons, you have photons, electrons and when we say molecules it is only limited to gases.

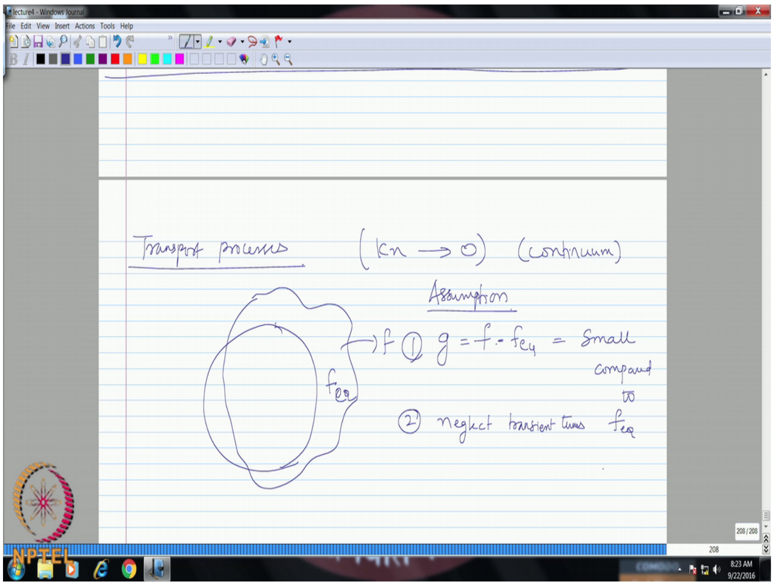
Therefore, these are applicable to plus gas molecule. So, if you want to simply use Boltzmann transport equation for liquids, then it is not valid. So mainly because, these fall under the dilute systems, and liquids are not and also you have strong intermolecular forces in liquids which are quite different from what we considered in the case of ideal gases using the kinetic theory and so on. Therefore, what happen when you want to go to liquid molecules, there are some alternatives? So, we modify the collision.

In fact, maybe the Boltzmann equation on the left hand side the advection part can be retained, but the collusion is to be modified to account for the more complex intermolecular interactions and the resulting equation sometimes people refer to as the en Enskog equation, and this can be used to describe the liquid molecule transport or more fundamental level you do molecular dynamics, which assumes an interaction potential between the molecule and this is also only the classical Newtonian equation f equal to ma.

In that case, you kind of capture most of the dynamics between the molecules and associated transport also can be captured. So, the 2 options that are available with dealing with liquid molecules are fundamentally, either you do a molecular dynamics or the Boltzmann equation can be modified the collision term can be modified and this is called Enskog equation. So, most of the discussion therefore, using Boltzmann equation is all limited to for example, solids where we are dealing with phonon and electron transport if you are talking about radiation transport here you can use Boltzmann equation and also system of gas molecules.

So, these are some of the, you know important limitations that you should understand. Apart from that you know this works reasonably fine, if you want to compare some results of the transport solution from the BTE with experiments. So, the BTE is even with the relaxation time approximation is found to be quite adequate and accurate in capturing all the physical phenomena.

(Refer Slide Time: 10:08)



So, with that we will move on to the actual transport process. So, the first case that we will consider will be the no low notes the number case. So, that is, so, let us move on to transport processes. So, we are going to first look at a limiting case, where we will try to derive the continuum constitutive relations such as the Fourier's equation the Fick's law ohms law Newton shear stress law and so on. So, how can we derive this from the Boltzmann transport equation? So, this is one case where we can find the analytical solutions quite comfortably. So, what we will do is once again. So, if you are looking at an equilibrium distribution function. So, let us call this f naught or f equilibrium what whatever you want to, and then from this you have a deviation which your actual non equilibrium distribution function f. Now if you want to derive the continuum equations, how much should be this deviation of f from f naught should it be large or should it be small?

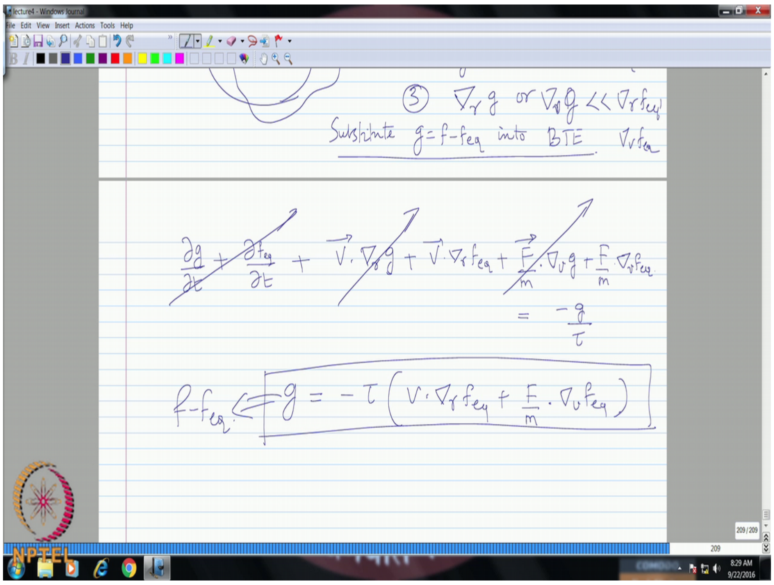
Now, you go back to what we did yesterday, in terms of Knudsen number and even one step before that f minus f equilibrium is equal to c power minus t by tau. So, when we are talking about large values of t by tau. So, this is the typical case of small notes and numbers right. So, in that case what would be the deviation of f from f equilibrium it will be very small right. So, therefore, in order to derive the continuum equations. So, we have to bring in the assumption that I have an f minus f equilibrium that is the difference between these 2 distributions, one is the equilibrium which is uniform in all the directions the other one which is non uniform and; however, this difference let us call this as another parameter this should be function g.

So, this will be small; therefore, when you say small relative to what, small compared to your equilibrium function. So, this is number 1 assumption that we are going to make. So, as you can see we cannot directly solve the BTE, the BTE if you look at the nature of the Boltzmann transport equation. So, we cannot find a direct analytical solution to this. So, therefore, we have to make certain assumptions under which we can try to find the analytical solution. So, this has to be solved numerically strictly speaking this is an integral differential equation; that means, it is a differentially partial differential equation and f equilibrium we can write this as you know integral of your certain distribution function.

So therefore, this becomes an integral differential equation and we cannot find a simple analytical solution to this. So, therefore, we have to bring in these assumptions. So, one of these assumptions is low Knutson numbers your deviation from the equilibrium is quite small. The other is that, when we solve the transport in the continuum cases such as the Fourier's law and Newton shear stress law these are all steady state processes you do not essentially have to consider the change with time. So therefore, we can neglect the transient terms. So, this is another important condition.

Therefore, now if you introduce this distribution g equal to f minus f equilibrium and you substitute. So, therefore, in place of f in terms of g, so, you go back to your BTE. So, rewrite your BTE now in terms of g and f equilibrium.

(Refer Slide Time: 15:18)

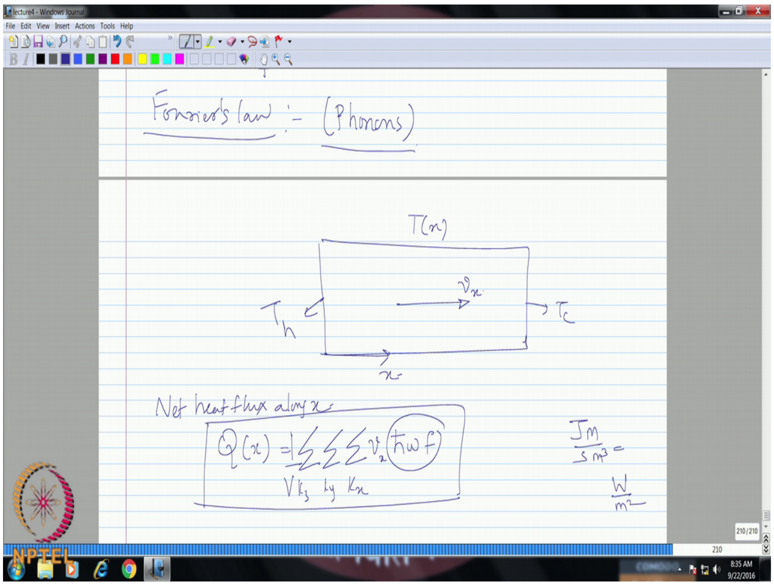


So, you have what are the terms you will have on the left hand side. You have d g by d t. And then, plus d f equilibrium by d t right, and then plus your v vector dotted with del r g right plus v vector dotted with del r f equilibrium plus you have your force by mass dotted with del v g plus f by m dotted with del v f equilibrium this is equal to on the right hand side, minus g by tau right, solving for is not just the secular distribution function, but the deviation from equilibrium right. So, we have cast the BTE for the deviation from the equilibrium.

Therefore, as per our assumptions neglecting transient terms, so, these terms are gone and we are also saying assume g is small compared to your f equilibrium and not only that the gradient of g should also be small, if g is also small that is not sufficient the change of the distribution function in either the physical space or in the momentum space should be quite small compared to the relative change that is happening to the equilibrium distribution function right.

So we can also bring in another assumption that gradients either when you say del r g or del r del v g should be smaller than del r f equilibrium and del v f equilibrium. So, under this, we can also neglect the other terms involving gradient of g. Finally, what we get is a relationship of g as minus tau times v dotted with del r f equilibrium plus f by m dotted with del v f equilibrium. So, this is your expression for the deviation function and now depending on the scenario we can plug this you can rewrite this as for example, f minus f equilibrium or in other words its tell it tells you for the limiting case of Knudsen number going to 0 what is the relation between the non equilibrium function f and the equilibrium function. So, this is your particular relation.

(Refer Slide Time: 20:37)



Therefore, once you express your non equilibrium function in terms of equilibrium, it becomes easier to solve them. Because you already know what the equilibrium distribution function is right. So, it becomes easy to solve. So, we will therefore, first take the case of deriving the Fourier's law that is heat conduction. And so, in the case of heat conduction, we can consider a domain where you have a high temperature on one end let us say t h and t c and there is a temperature variation along x which is this direction right. And now, if I want to calculate what is the heat flux from the non equilibrium distribution function. So, earlier from the kinetic theory if you remember we also calculated heats flux right.

In that case we looked at the interface we looked at what is the flux going in one direction minus flux the opposite direction. So, the net flux was the net heat flux going in the positive x. So, now, directly we want to calculate the net heat flux along x. So, now, we want to use the distribution function f. So, how do you how do we, in this case do that. So, we have to consider for example, phonons; let us assume that this has phonon gas and therefore, the energy of each quantum state can be assumed to be h bar omega and the distribution function non equilibrium distribution function now is denoted with by f right. So, each quantum state is occupied by certain number of phonons. So, and the energy of each quantum state is h bar omega. So, therefore, what does this give you h bar omega time's f?

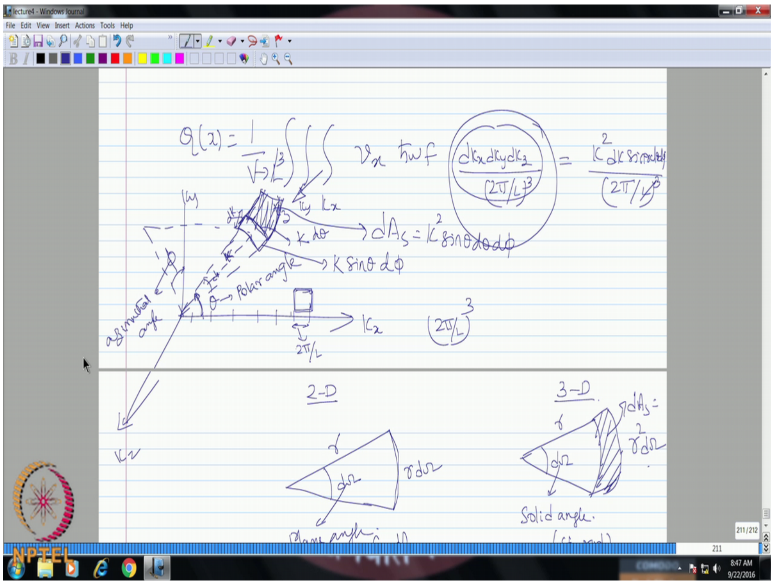
Student: (Refer Time: 23:04).

This just gives an energy distribution therefore, to calculate the total energy. Sum it over all the states. So, if you are looking in terms of wave vector space, because you when you say momentum space momentum space is also nothing but wave vector space, you can write this f by m del v s f by h bar del k. So, they are all similar. So therefore, all this can be summed over all the quantum states possible the wave vector space and this gives you only kind of the total energy, but what about the heat flux. Now flux is a quantity associated with motion heat flux. So, we did this when we did statistical thermodynamics only difference was, we used an equilibrium distribution function there and this gave you the total internal energy of the system, but now we are interested in flux which is associated with the motion of the phonons with a given velocity right.

So, let us say the velocity is some v x the phonon transport, the phonons are moving with a velocity v x. So, therefore, how do you calculate the flux based on this? So, what will be the unit of this set let us say, this is now joules I want to convert this into watt per meter square. So, into velocity, so, this will give you a joule meter per second, divided by the volume. So, this will now give me what per meter square. So, I consider there for a domain with volume capital v and I look at the velocity of the phonons along the x direction that is v x. So, that multiplied by the energy distribution and sum this over all the quantum states is going to give me the net heat flux along x. So, everybody agrees.

So, this is now the common thread for all the transports loss, if you want to now study Fick's law. So, you will instead of energy flux we will consider these mass flux, but it is evaluated in a similar fashion if you are considering now ohms law. So, you will consider charge flux. So, minus e times f so, this is a common expression, therefore, if you understand this the same thing, can be extended to describe other energy carriers. So, now, what we have is a discrete summation right. So, we have to convert once again this discrete summation into an integral in order to evaluate it. So, we are now saying we are summing this overall the quantum states represented by k.

(Refer Slide Time: 26:42)



Therefore, if you want to convert this into an integral, overall the wave vectors we have v x h bar f. So, we should therefore, have a d k x d k y d k z z divided something because, these are conversion from the numbers to an integral. So, this should therefore, be represented by some number, that is the number of quantum states correct. So, therefore, how do we calculate this? So; that means, if you take the case of 3 dimensional wave vector space, so, let us say you have k x k y k z all right. And assume that you can have some kind of a scaling you can break this down into smaller scale such that the length minimum length of this will be equal to 2 pi by l.

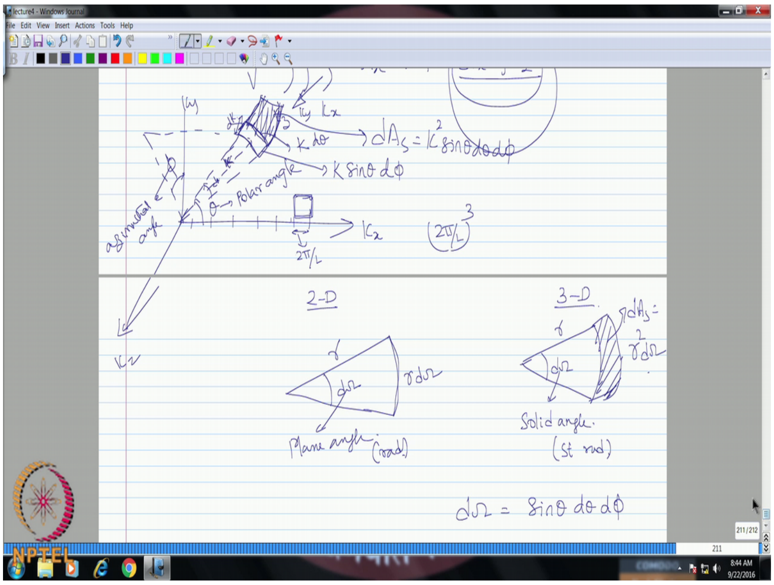
So, the volume of each of these unit sub cells, in the space of k x k y k z will be 2 pi by l the whole cube. This concept, we used in defining the density of state right. So, now, what we are interested is if you want to have a sphere a solid sphere in the k x k y k z space, and I am now counting the number of quantum states within the sphere. So, how will I get this? So, I have to calculate the volume of the sphere and divided by single unit cell. So, that is 2 pi by l the whole cube. So, therefore, you can imagine now. So, I will have piece of a sphere a portion of a sphere now. So, which I can now if I integrate it over the entire momentum space will now give me a total solid sphere.

So, how am I going to do this, if you if you look at from this projection. So, I will have sector like this so; that means, I have k vector or k and this is d k and the angle that this is making with the x is given by the angle theta, and now if you project this particular k on to the y z plane. So, this projection will make an angle of fee with the y axis. So, these are the spherical this is a spherical coordinate system right. So, this is the 3 dimensional spaces and its multi directional; that means, you can have any values of wave vector which can be aligned in any direction.

So therefore, we have to consider a three dimensional spherical coordinate system. So, what we have is in terms of radius we have the magnitude of k and we have theta; this is your polar angle and phi will be your azimuthal angle. So, the projection of this on to the y z plane will make an angle phi with the y coordinates. So, just to give a summary; so, if you take 2 dimensional sector. So, in this case, we have radius r and let us say the plane angle here is some t omega.

This is a 2 d case. So, therefore, the arc length here will be r d omega right, this is like a small slice. So, now, if you extend this to a 3 d, so, we are replacing this plane angle. On this projection, it will look similar with a solid angle and we still have r, but what will be the area of this. So, it will be r square do omega right. Now, the question is how do we calculate this angle? Now this angle is called solid angle whereas, in 2 d you call this as plane angle I hope you know the difference. So, this is your radiant and this is steradian solid angle ready steradian.

(Refer Slide Time: 32:53)

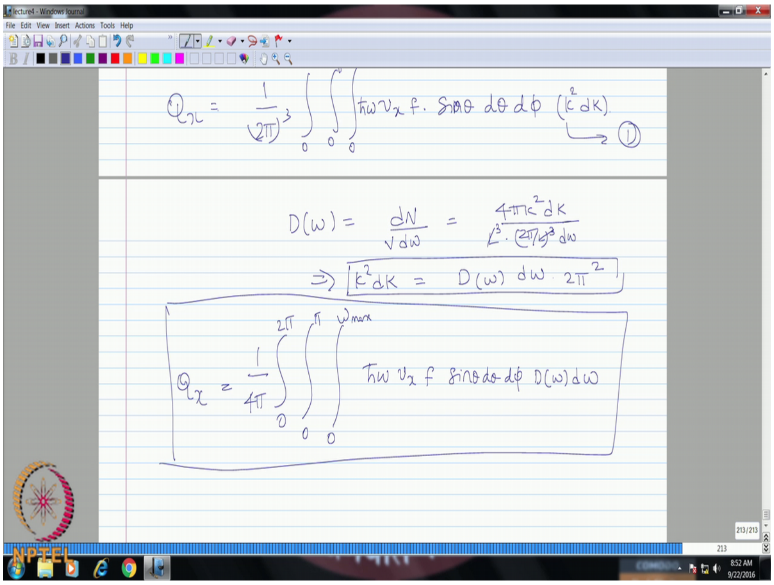


So therefore, the question is how do we calculate this solid angle? So, therefore, the surface area now d a s will be r square d omega. So, if you do some trigonometry, and you will be able to find out that d omega will be sine theta d theta d phi so; that means, what we are trying to do is find out. So, this is basically in this dimension, now if you are looking from observer like this. Therefore, you will be seeing something like this; we want to calculate this area. This area will be this multiplied by the projection of this on to the y z plane. Now, this here is your k into if you say this is your d theta here; this is your k into d theta. So, the other side will turn out to be k sine theta into d phi. So, that together the area of this subtended by the solid angle will become k square sine theta d theta d phi. So, that is what we have written here r square is nothing, but your k square here.

So therefore, if you want to calculate the volume, so, we have therefore, k square sine theta d theta d phi times p k right, that is the volume now if you integrate this for limits of k x k y k z ranging from zero to infinity you subtend a huge sphere now ranging from all the way from the center to infinity right. So, you are subtending a huge sphere. So, this is the sphere, where we are now concerned about finding all the quantum states counting the number of quantum states with in this entire solid sphere. So, therefore, when we are replacing this summation discreet summation with an integral therefore, we have to now say d k x d k y d k z divided by 2 pi by l the whole cube. So, this will therefore, give me the total volume of this entire sphere divided by 2 pi by l will give me the number of quantum states. Therefore, this is the way I have to convert a discrete summation into a integral. Now my d k d k by d k z what I have found out is nothing, but the volume of this subtended by the solid angle.

Therefore, I can rewrite this as k square d k into sine theta d theta d phi divided by 2 pi by l the whole cube right, and therefore, what is the volume here, l cube a total volume. So therefore, by l cube and l cube here cancel off right. So, I can now rewrite now you look at the integrals in these original integrals are in terms of k. So, I have to convert this in terms of theta and phi right, so, in terms of theta and phi. Now if I want to make this a sphere. So, what will be the limit of theta and see my theta should go from zero to pi and then phi from 0 to pi by 2 and phi from 0 to 2 pi right. So, this will be, so, this will be 0 to pi. So, this will make a hemisphere.

(Refer Slide Time: 37:58)



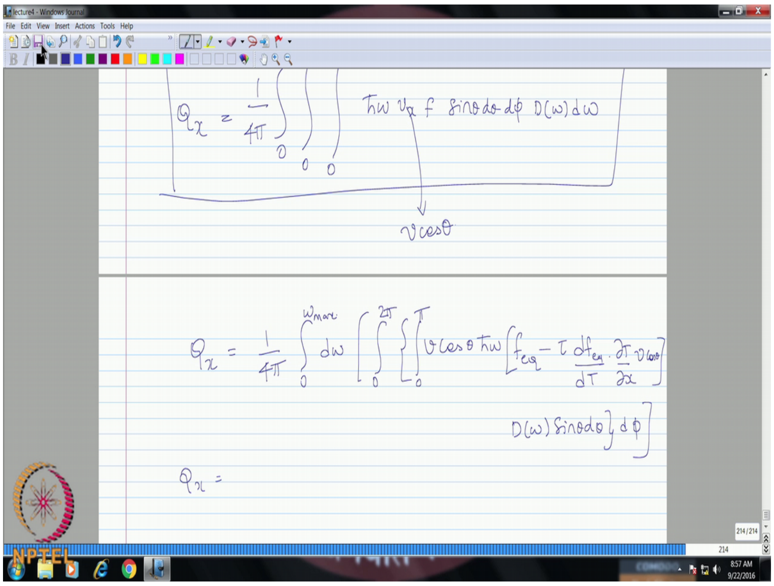
So, it has to go from 0 to pi. So, I will make 1 semi circle which I rotate about the x axis by 2 pi times, so, to make a complete solid sphere. So, therefore, when I convert this to the theta phi space, so, what we are doing is essentially, we are converting the k x k y k z to a spherical coordinate system theta phi. So, therefore, the resulting expression for q x now will have one by 2 pi the whole cube and. So, I have integral please make sure I think this is. So, we have 0 to pi for theta and 0 to 2 pi and then I have for omega I have from 0 to should be 0 to omega max, which will be the d by frequency the maximum 1 and I will have a v x into f into sine h bar omega into sine theta, d theta d phi and I have k square d k.

So, I think. So, this is this is the expression now the thing is, I have to completely convert my k square d k in terms of omega. So, I have already changed the limits here because, I have h bar omega. So, I have to convert my k square d k to omega. So, how can I do that using the density of states? So, now, the expression for density of states, his number of states per unit frequency interval per unit volume is the density of states per unit volume. So, that is number of states if I take one annular strip of a sphere. So, I have the surface area for pi k square b k right. So, this will be the volume of the annular strip divided by two pi by l the whole cube and I have the volume which is l cube d omega right. So, therefore, from this I can what is the expression for k square b k in terms of d omega my l cube cancel off here.

So, I should be getting d of omega d omega times 2 pi square right, therefore, please substitute this into let us say, equation 1 for d square k square d k. So, you will have q x therefore, will be so, you have 2 pi square you have 2 pi the whole cube. So, therefore, this will be 1 by 4 pi right, and you have 0 to pi you have 0 to 2 pi is phi 0 2 pi is your theta and frequency 0 to omega max h bar omega v x into f into sine theta d theta d phi into d of omega d omega, I hope all of you understood till this point. So, what we have done essentially, is first started with the discrete summation over the wave vector space, and then converted that into a continuous integral over the solid angle theta and fee and again we have a k square d k now we are converting k in terms of omega that is all finally, so, using the density of state. So, therefore, now my d k x d k y d k z is replaced with 0 to omega max 0 to pi 0 to 2 pi.

So, this is how I can convert my wave vector space into a physical space you understand. So, my theta phi these are physical coordinates my k x k y k a z they are momentum space. So, how do we convert momentum space to physical space is using the density of states right. Now once I get this expression, I can now plug in what I have for f' that is the generic thing right f minus x f equilibrium is equal to this. So, I can plug in my expression for f from this now first if you are looking at only heat transport. So, there is no external force term. So therefore, this part will be 0 right there is no gradient in the momentum due to the external force. So, that part will be 0, therefore, now if I substitute that into this equation.

(Refer Slide Time: 44:43)



So, I have q x will be 1 by 4 pi and I am going to separate out the frequency integral and the solid angle integral. So, I am just going to rewrite it 0 to omega max into d omega, this is the outer integral. So, I have then 0 to 2 pi and the innermost integral will be the 0 to pi this is your polar angle. So, my v x now will be in terms of theta v cos theta right. So, in the direction of this k is my v momentum basically or velocities in the same direction. So, therefore, I can write my v x as v cos theta. So, I can convert everything to a physical coordinate. So, we cos theta into h bar omega, now for f I substitute from the above function tau I have d f equilibrium by d x. Now, I am considering only one dimension.

So, my del, del r f will become d f equilibrium by d x which now I can write this as d f equilibrium by d t, because f equilibrium is a function of temperature right, if you take the Bohr Einstein distribution function into d t by d x and again I have a v x there right. So, dotted with v x. So, if you look at this, so, this in one dimension is nothing but v x times d f equilibrium by d x. So, I can again write this v x as v cos theta and d of omega sine theta d theta because, that is your inner integral theta ranging from 0 to pi and then the outer integral is d phi outermost is d omega.

So, let me quickly complete this. Therefore, if you probably will stop here, because I think we have a few more steps and we do not have enough time your next professor is waiting. So, you just maybe go home and once again re derive till this part. So, that you are confident and then the other steps are there are couples of steps after this to reach the Fourier’s law we will stop here.