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Lecture - 26 Derivation of Continuum Laws from Boltzmann Transport Equation Part 3

(Refer Slide Time: 00:20)

Good morning. We will complete the exercise on the Ohms law. Derivation of Ohms laws from the Boltzmann Transport Equation. I hope all of you are able to go back home yesterday and try to rewrite some of the steps, I think very similar to the phonon transport except; that when you take the derivative of the equilibrium function, with respect to x, we have to make sure now, that we have gradient of the Fermi level, e f rather than the temperature that was there for the forum transport and the other thing is that, we have an electric field due to the transport of electrons and that also has to be included because of the Lorentz force.

The essentially, the change in the gradient in the equilibrium, with respect to the momentum space or the velocity space also has to be accounted for through the dependency of the energy on the momentum or velocity. So, we have therefore, expressed our derivative d f naught by d x, as well as d f naught by d v, in terms of you know dependency of Fermi level on x and also the energy on v x. So, therefore, we have a additional term compare to what we had for the phonon transport.

(Refer Slide Time: 02:02)

That was the term, which is the term e f and there be no transport of charge or current. So, this electric field term; would have been 0 and this would have looked similar to the phonon transport and if there was only temperature gradient then instead of dE f by d x; you would have d t by d x correct.

With this additional term therefore, we now have the generalized form of the Ohms law which is applicable equally for both metals and semi conductors.

However, when we are now focusing on metals, we can make an approximation that, the number density of free electrons are already too many and assuming that, the change in the Fermi level is not too large with position therefore, we can neglect the gradient d f by d x and therefore, we get reach the point where we can write down the Ohms law for the metallic materials. If you want to cast it in the classical form of Ohms law, we have to therefore, relate it to the property called electrical conductivity. Therefore, this is your classical form of Ohms law. Therefore, we now get a relation to estimate electric conductivity from, the Nanoscale transport process.

The Nanoscale transport process here involve, the dependency of the equilibrium distribution function on energy as well as the relaxation time, velocity of electrons, density of states for electrons and so on right. We can also do a further simplification of this.

For example if you once again go back to the Fermi Dirac distribution function. Which is relevant for electrons and if you look at how the occupancy distribution looks right. So, about the Fermi energy level e f, you can say this is your chemical potential at 0 kel right. You have for example, certain distribution of electrons; now below the Fermi level and few above the Fermi level and therefore, if you are really plotting this at 0 Kelvin this would be a, sharp cut off, it is a direct delta function. Whereas higher temperatures you have a gradual occupancy.

All the lower energy levels are first occupied and then beyond the Fermi level also there are electrons present. These are the free electrons now which can move around and these are the cost for the high electrical and thermal conductivity of metals right. Therefore, if you want to calculate the derivative d f equilibrium by dE, you will find that the derivative usually has finite value around the Fermi level whereas, if you move away from the Fermi level. So, that will be 0 because they are usually flattened out, so unless you are looking at very high temperatures. At very high temperatures, then this curve will gradually become straight line. There we cannot make this assumption, but at moderate room temperature and so on.

Low temperatures; we can make an assumption that therefore, d f equilibrium by dE is non 0; around the Fermi energy level. We have already made this assumption once before; in deriving the heat capacity of electrons. If you put this assumption therefore, the integral term of d f equilibrium by dE, says that I mean only around e f, this value will be finite and non 0 and other regions; it will be 0 and if you integrate therefore, d f equilibrium. It should therefore, satisfy from values of energy 0 to infinity, it should be one basically. So, if you integrate this with respect to d e, you know then it should make sure that maximum value is 1, minimum value is 0 and therefore, this can reduce to the form minus e square by 3. So, the value of a tau at Fermi level, we have velocity at Fermi level. You have the density of states also at the Fermi level. We are now making simplistic approximation; where in all the derivatives at different locations can be ignored and only, we are looking at evaluating the integral at the Fermi level.

At the Fermi level you take all the values corresponding to the Fermi level and you simply take them out as constants and integrate d f by dE d and which turns out to be 1. Because this is has to vary from, the value of f equilibrium has to vary from 0 to 1 overall. in this case; the reduction of expression for thermal conductive happens from this to this form. So, we will call this as equation number 2 and this is mostly the form that is used to evaluate the electrical conductive of metals. That means, you use directly the density of states evaluated at, the Fermi level e f into this expression. The corresponding relaxation time, the relaxation time can be assumed to be constant independent of the energy level. And we can also assume the velocity of the electrons to be constant. In that case, we can directly evaluate dE f substitute in to this and therefore, you get the expression for the electric conductivity right.

This is similar again, if you go back and refer to the expression for thermal conductivity. What did we have? We also had tau v square and C. C v divided by 3. Except now, we instead of C v; we have something like e square times, the density of states. Here also, the C v had a density of states. We assumed suppose; if density of states can be integrated assuming tau and v are constant. We get the total volumetric heat capacity. There is analogy between the ways the electrical conductivity and thermal conductivity are related to the relaxation time and the velocity of the energy carriers. So, this is to give 1 example. If you for example, yesterday we were talking about the case, where you can also have simultaneous transport of charge flux and it can also transport temperature. That is a case, where you have a non isothermal surface. So, in that case you also have a temperature gradient along with the electron flux.

(Refer Slide Time: 10:26)

Therefore, how do we evaluate in that case. So, this is usually the case when you consider the thermo electric effects; that mean, you have a semi conductor or metal. You have a d t by d x and you also, have the change in the electro chemical potential gradient. There is an electro chemical potential gradient, you have a temperature gradient when you want to therefore, calculate our d f equilibrium by d x. So, the same expression is still valid for this case f is equal to f equilibrium minus tau v x into d f equilibrium by d x and so on. Except that now, d f equilibrium by d x can be written as d f equilibrium by dE into dE by dE f by d x right.

You also can write this as d f equilibrium. We can write this as partial derivative here d f equilibrium by d t into d t by d x. So, now, you have an additional term which accounts for they also transport of heat; along with the charge transport. Now, you therefore, have to plug this into the expression here. Let us call this 1. In place of this you plug. There we had only dE f by d x; now we also have the second term which is the temperature gradient term and then proceed. Therefore, this is much more complex expression then, when you consider without the temperature gradient or without the charge gradient. But never the less; what this tells you, we can also do a similar procedure to calculate for example, the c by coefficient. For calculating into understand, for given temperature difference how much is the current actually produced and similarly Peltier coefficient which is the other effect you pass the current and then; you can basically maintain as a result temperature difference.

You can basically transfer heat from a colder side to hotter side; which requires a work input according to second law of thermo dynamics right. That work input here is the currant. This is used in the Peltier effect. Therefore, we can get expression for both the Seebeck and Peltier coefficients. So, I am not going to do this now, but if you are interested you can refer to text book and I think in the test book this has been derived. With this, you know all these are things which probably, you know for the micro scale point of view. Now we know how, now we have to use thermal conductive electrical conductive and similarly if you want to do this for molecules.

(Refer Slide Time: 14:05)

So, we are talking about ideal gas molecules right. We can derive the Newton's Shear Stress Law. Where you want to say that tau x y is the shear stress, is related to u d u by d y. Now, this is going to be a little bit more straight forward; only I will give the Maxwell

distribution. So, this can be derived for a scenario, where we can again talk about flow between 2 plates. The top plate is moving this is the called the couette flow ok.

The top plate is moving with a velocity U, bottom plate is fixed and steady state velocity profile; turns out to be a learner profile like this. 0 at y equal to 0 and at y equal to let us say H, which is the separation between the plates. It attends the velocity of the top plate U and you have your molecular velocities; v x and v y and similarly in the third direction you have v z right.

(Refer Slide Time: 15:39)

For this case, the Maxwell Boltzmann distribution function; will be looking like n into m by 2 pi k b t the whole power 3 by 2, where n is the number density of gas molecules number of, total number of molecules per unit volume. m is the mass of the molecules and we have e power minus m. Now, in the classical Maxwell Boltzmann; we have v x square plus v y square plus v z square.

That is the translational kinetic energy. Assuming these are all only mono atomic gas molecules divided by k b t right so; however, now since we also have a flow right. We do not, not only have a random motion of the molecules, but also bulk motion of these you know gas molecules in a certain direction. So, in this case we can say that, the bulk

velocity in the x direction is u; which is a function of y this is the velocity profile. For the couette flow u of y will be U into y by h.

It is a linear profile. If it a poiseuille flow, in a circular duct then you can put the parabolic profile and so on. But never the less; the classical Maxwell Boltzmann distribution, does not account for basically the bulk motion. We have to therefore, correct this. Therefore, the velocity, will become v x; which is your molecular velocity minus u of y, which is your bulk velocity the whole square. Where as in the other directions, there are there is no bulk velocity therefore, you have only the molecular velocity divided by 2 times k B t. So, this becomes what is called as the displaced Maxwell Boltzmann distribution.

This is usually used, when you are talking about flow transport. When you are talking about statics; then you use your conventional Maxwell Boltzmann. When you talk about bulk motion; then in term you replace that with the displace Maxwell Boltzmann. Simply, wherever you have the velocities you have to correct it, by the difference between your molecular velocity and the bulk velocity and this is now used.

You again have the relationship between f and f equilibrium minus tau into v dot del r f e equilibrium. The force term is 0 here correct. Now, we have to evaluate this. You have f e equilibrium minus tau and this is your molecular velocity here. This because please remember; this is the velocity of energy carriers, not the bulk velocity right. Therefore, this will be v x. We have v x, v y, v z; however, when you talk about the gradient or derivative of f e equilibrium. Your f e equilibrium; now can have gradients in all the 3 directions, but in our case in which direction it is going to be significant.

Student: Along y.

Along y because this profile u is the function of y therefore, when you want to express d f equilibrium by d x, along d x, there is no variation. Because I mean u x, u y, u z are all constants whereas along y, your bulk velocity profile is the function of y. Therefore, this we have to be careful; when you take the dot product of this. So, we have v x, v y, v z and therefore, this will become v x times d f equilibrium by d x, which will be 0. I plus you have v y into d f equilibrium by d y j and since this gradient is 0 along x therefore, only this has to be retain. You have f equilibrium minus tau v y into b f equilibrium by d y.

Now, d f equilibrium by d y can be written as d f equilibrium. So, what is the function of y? Only u is the function of y. It related to u and u have d u by d y. So, this can be substituted to calculate; your shear stress, now the expression for shear stress becomes much easier.

(Refer Slide Time: 20:55)

Because Maxwell Boltzmann distribution is a continue distribution. You do not sum them over, but you directly integrate them. So, therefore, you directly integrate them over all; d v x, d v y, d v z right. Over the entire momentum space, you directly integrate. You do not have do a conversion involve density of states and all that here.

How will you calculate the shear stress? It is like; it is nothing but flux of momentum right. Momentum flux is nothing but shear stress. In this case the momentum flux; you are talking about the flux of x momentum right. In which direction, y direction, therefore, we have the x momentum, which is m v x; however; the flux will be in which direction y. Therefore, we have to multiply it with v y and the corresponding non

equilibrium distribution. Therefore, this has to be integrated over all the through the entire momentum space; we have v x going from minus infinity to infinity v y and v z. So, this can be interpreted as therefore, the momentum flux per quantum state. Which you are now integrating over all the quantum states, the quantum states; however, we cannot say quantum state in for the gas molecules.

Because they are all continues distribution functions. These are nothing, but the entire momentum spaces, which is continues. If you take one small chunk, may be d v x, d v y, d v z. So, you have a particular flux of momentum. And if you integrate this over the entire once again conceptualize like spherical coordinate system; you get the total momentum flux. And this momentum flux is nothing but the flux of x momentum which is going vertically upward. This is the flux of the x momentum in this direction.

This is what we want to calculate to relate to basically calculate the shear stress tau x y. Because, we know that this, tau x y has to be relate to d u by d y. So, which is basically nothing but the expression of the flux of x momentum in the vertical direction, gives you the stress on the shear stress on the bottom plane. You can do a similar analysis like, we did for phonons; all you have to substitute now is the expression for f from this into this. You can evaluate d f equilibrium by d u; basically you can differentiate it with respect to d u and similarly d u by d y. Because d u by d y is known for the couette flow and I will give only the final expression.

If, you do all that; you can express tau x y as sum the mu into d u by d y in the form; which is classically known, where mu will come out to be 1 by 4 times d square, square root of m k B t by pi.

I will leave this, as an exercise for you to substitute and integrate this. You can do this integration in mathematical. d is the diameter of the molecule. Now, how this we got is you remember. We have actually the expression in terms of the relaxation time, but we can rewrite that in terms of mean free path and we have already derived the expression for mean free path in terms of diameter of the molecules. We can substitute that and finally, get a very fundamental expression.

In terms of temperature, in terms of the mass of the molecule, in terms of the diameter of the molecule, and if you compare this again with your expression from kinetic theory, it will be similar. If you go back and rewrite that expression, the expression that we derived under kinetic theory again; we need to substitute for the mean free path. You can go back and refer to that expression; you can substitute for mean free path and finally, you will get the same expression here. Is that clear?

So, therefore, using the Boltzmann transport equation, with an assumption that you know the deviation from equilibrium is very small. We have shown that we can derive all continue constitutive relations. All of them almost, you can also derive the fix log diffusion in the similar manner. When you, if you want to talk about therefore, mass transport, momentum transport, heat transport, charges transport, these are the 4 main most important transport mechanisms. That is dealt with by mechanical engineers by chemical engineers, electrical engineers. All of this can be shown to obtain from fundamentally from the Boltzmann Transport Equation.

This one thing and I want to quickly summarize, summarize and conclude; what we can basically take away from using Boltzmann Equation for deriving the Continuum equation; however, we have to also look at the validity of the Continuum Equations themselves. Already, I have given you, some indication that, there are problems when you apply them to slightly higher Knudsen numbers. But let us try to understand, what the physical bases of this are. It is a generally talked about in terms of Knudsen number, but what happens? What really gets violated? When you apply the Continuum equations to large or moderate Knudsen numbers; to illustrate it once again we will go back to the assumption that we made in deriving all these Continuum constitutive relations.

(Refer Slide Time: 28:29)

We always assume your f equilibrium to be independent of the directional space and we therefore, took another distribution, which is the actual non equilibrium distribution and the deviation between these 2 right. Now this is going to be the indicator of the extent of the local non equilibrium. So, this is your at your particular location x, we are talking about your deviation of f from f equilibrium.

So, the higher the deviation, the more is the indicator of local non equilibrium which means that more is the deviation from making a Continuum assumption. Therefore, we use this function g to indicate how far your f is displaced from your f equilibrium. We made an assumption that number 1, that your deviation is substantially smaller than your actually equilibrium distribution function itself. This is the basis of deriving all the Continuum equations right.

So, and number 2 also the gradients, whether you are talking about the momentum space or the actual physical Space. The gradients of the deviation function are actually much smaller than the equilibrium gradients. This is again an important assumption that (Refer Time: 30:36) to eliminate all the derivatives involving g. And also, we made another important. Therefore, as we can also say that, we can also look at the time scales on 1 hand you had for example, d f equilibrium by d t and you also had d g by d t and on the right hand side; you had your f equilibrium minus f which is nothing, but g by tau.

So, we also neglected these terms with respect to the right hand side. We said, we are looking at study state. But even when you are looking at unsteady process; the order of magnitude of these terms for the Continuum processes, can be found to be smaller than this term. For example, if you are saying d g by d t, it is much smaller than g by tau. So, therefore, since we are claiming that the order of g and order of b g is similar. So, therefore, we have to say that, the physical time scales t will be much greater than your relaxation time tau right.

In order for this assumption to be valid what this means? You know do not, not only have problem with Knudsen numbers. So, there can be a case were, a you can have value of Knudsen number equal to 0.001; that means, it is going to satisfy this condition and this condition, but still that can violate this third condition. How because you can have time scales, which are much smaller than the relaxation time, it is a good example of this will be for example, if we have a laser pulse which is basically irradiated on a surface. It could be a metal or semi conductor. So, we are talking about this pulse width of the laser.

So, if you have a pulse lasers. So, usually pulse lasers are used in machining processes and so on. You have continuous lasers, you have pulse laser, but pulse laser have specific applications, where you want to make some deformations on the surface. You want to (Refer Time: 33:32) out some material and so on. This pulse width can be very very short. So, if you are talking about a picosecond laser; that means, the pulse width is of the order of 10 power minus 12 seconds. And similarly, we have up to femtosecond lasers. It is a pulse width is of the, order of 10 power minus 15 seconds. You just give a pulse, which is of that width and you let it go.

Now this pulse comes and hits the surface; now what is the order of mean free path? If you are talking about phonons for example, just the order of magnitude; you have done some calculations in your assignments. So, you should be able to tell me. Let us say silicon; semi conductor material. 1 nanometer is very small. It should be of the order of 22 few 100 nanometers. Even if you say 20 nanometers if you are talking about electrons; then that can be the order of few nanometers.

But generally all this relaxation time scales of the order of nanometer. Now, when you use picosecond or femtosecond laser what happens, this condition is violated. Clearly therefore, you are talking about Knudsen number which is perfectly seems to be in a Continuum range, but the third condition is clearly violated so; that means, still you cannot make this assumption for this case to derive the Continuum equation. This is clearly not this is not your Continuum.

Therefore, you have to be careful, when you judge. What is sub continue? Not only the length scales, but time scales are also very important because to derive all these Continuum equations, from fundamental Boltzmann transport equation. We have to list down the assumptions we make and one of the assumptions is that your physical time scales are much larger than the relaxation time scales and if any process which violet this will not satisfy Continuum right.

This is the very very important thing and I mean to highlight this, how we ignore this, many times when we even derive you know heat transfer laws. Just to give an example, because this is a good example also given in (Refer Time: 36:39) test book. I find that many people may not even understand, that they are violating. This is actually, the case were we talk about no I think many people would have done this. In the heat transfer, we derive the semi infinite approximation in conduction, transient conduction. How many of you remember the transient conduction problem? In transient conduction what we say is there are different ways of dealing transient conduction. We have small biot number cases; we have a moderate and large biot number case that is one thing. And we have another case for example, if you take entire earth we do not want to spend time in solving conduction, right from the core of the earth to upper layer. So, that is impossible to do right.

You are talking about several thousands of kilometers and finally, if you go and measure some point here. So, this temperature will be quite different from this temperature. Assuming that, some I mean, we do not have any source of energy at the core. If you apply some heat at this point, let us say you maintain this as T wall. If you consider the other end; which is may be several thousands of kilometers. Within few seconds or minutes this will never be able to sense this temperature correct. Therefore, this will be at whatever initial temperature it is there.

We do not have to solve a transient conduction rigorously through the entire body. So, we make an assumption that the other end is always static; so that means, the initial condition is imposed on the other end as a boundary condition. So, this is always at the initial temperature whereas, you solve the heat equation only for say, what we called as half of the domain half of the domain and we impose this condition to the other end whereas, the this end is where we impose the physical temperature, higher temperature or a heat flux or a convection boundary condition.

And when we solve this typical, the transient heat conduction, which all of you know. So, d T by d t is equal to you have alpha k by rho c p. So, we can write this as basically alpha times d square t by d x square. If you are talking about heat conduction in this direction and with the boundary conditions that at x equal to 0 you have T wall and at x going to infinity. It is at the initial temperature t i.

The solution that comes out will be $T x$ comma t will be an exponential d k minus x divided by square root of alpha t, is of this form. You have some other constants but basically it is an exponential variation. What it tells is that, if you apply a temperature pulse for example, here momentarily and then live it. According to this, now this expression is of course, we already use the Fourier's conduction equation here right. And then we are deriving this equation for temperature. So, what it say that x going to infinity what is a value of temperature.

So, let us say this is something which is quite large. Maybe something like 100 kilometers or something like that. So, if you plug in the value of x; this value of temperature according to this equation will not be exactly 0, but it will be some finite value right. Even a momentary pulse this does not distinguish, whether you have a picosecond pulse or you are continuously heating. So, whatever you apply. So, this says that at position which is very very large.

So, there the value of temperature is still finite means, that it is assuming that the speed of propagation of heat is not equal to the speed of sound in the medium, but it is infinite. The moment you apply basically a temperature or a heat flux on one end and immediately other end is able to sense it and response to that. Which is, which we know now, from the basic energy carrier point of view that cannot be possible because the energy carriers in this case, it would be phonons or electrons are traveling with the finite speed.

And many a times, if you are talking about femtosecond or picosecond irradiation; we cannot even by the time it even senses the I mean incoming radiation basically you have the impact. They cannot even transfer this. Therefore, you get hot spots. Suddenly you get portions, which are having very high temperature; because the local electrons are too excited, that they cannot even transfer the energy to the neighbouring electrons, but simply they explore with lot of heat; however, if you use the Fourier's equation it is very clear that it tells you that the speed of propagation of this heat is infinite and the other end is still able to sense some finite value of temperature.

So, this is a clear elastration of the fallacy of using the Fourier's constitute relationship; for a case where it is definitely not possible to no. In this case you definitely cannot except, if you put a thermo couple there, you will not be able to actually measure any temperature coming from the other end; but the distribution from the Fourier's equation shows its only exponentially d k right.

Therefore, what do we do for such cases? Where you have problem with, where the Fourier's law violates, but you want to still retain the Continuum based assumption. You do not want to completely discard the Continuum based assumption. The cases where you have extremely small physical time scales correct or you have problems with this kind of you know semi infinite medium and so on.

Therefore, we use what is called as the Cattaneo equation. So, this is called Cattaneo equation. The Cattaneo equation is a modification to the Fourier's equation; or it is a correction to the Fourier equation. So, basically your Fourier equation says that your heat flux is equal to minus k d T by d x. Now the Cattaneo equation puts a correction term to this, which is basically tau into d q by d t it adds the correction term.

So, what this tells you is that it now brings in a time factor. This is your relaxation time of the energy carrier. You see the Continuum equation themselves; do not talked about anything about the collision of energy carriers and so on. But without bringing that into account, you cannot talk about the finite speed of propagation of heat. So, therefore, to correct for that, we have a relaxation time tau. In the case of larger Knudsen numbers; you can talk in terms of large values of tau.

So, then this term become significant if you talk about the limiting case, where tau goes to 0. So, this can disappear vanish and you get your Fourier's equation right, but this is a correction term which accounts for the finite speed of the propagation of heat and if you substitute this into the heat conduction equation. Our heat conduction equation states that, your rho c d t by d t is equal to minus del dot q.

(Refer Slide Time: 45:47)

So, you can substitute instead of the classical Fourier's approximation, you can substitute the Cattaneo equation and you can derive, what is called the hyperbolic heat conduction equation. Resulting equation is called hyperbolic heat conduction equation. So, this is called hyperbolic, because of accounting for the finite speed of propagation. So, like any hyperbolic equation and this is used as a substitute in cases where you have problems with the time scales. So, any physical process which has smaller time scales than the relaxation time. So, we still may use the Continuum assumption, but we correct it with the Cattaneo equation.

Just with this I want to finish this part. Now also talking about, we are still talking about Continuum equation. So, the last part is. How do we really derive all the Continuum equations, there is conservation of mass, conservation of momentum, conservation of energy and so on. Because we showed that all the constitute relation, that is relating flux with the gradient we are able to derive, but what about the conservation of all the fundamental quantities like mass momentum and energy.

So, even this can be derived from b t e. Just to show that for example, you have your Boltzmann Transport Equation plus you have f by m dot del v f, if you take the moments you know. So, when we say moment, we have to multiplied with the corresponding quantity x. which is of interest for example, if it is mass you multiplied by mass, if it momentum, momentum energy and you integrate this over the entire momentum space.

(Refer Slide Time: 48:04)

So, we call this is d cube v and on the right hand side. So, on we have on the right hand side, the collusion term also which has to be multiplied by the corresponding quantity and you integrate it. So, your x could be mass or momentum or energy. It could be kinetic if you have monotonic gas, you can have kinetic energy plus, you can also have vibrational energy, potential energies and so on.

You substitute into this and we can integrate it over the momentum space. So, we will be able to see that, we can get all the conservation laws like, continuity equation, momentum equation and energy equation. Not only the constitutive relations, but also the conservation equations can be derived from the Boltzmann Transport Equation by talking the suitable moments.

I will probably put a small homework problem, where you can substitute for mass and then show that continuity equation can be derived from this. It is a quite straight forward. With that we will stop discussion related to application of Boltzmann equation to Continuum process. In the next 2 to 3 classes, we will derive use Boltzmann equation to derive the Nanoscale transport process. So, far we have not done any example where we have a high Knudsen number case and we want to see how for example, the temperature distribution looks. That is the last part of the Nanoscale transport. We will take that up, starting tomorrow another couple of class; we will derive the Nanoscale transport process.

Thank you.