Micro and Nanoscale Energy Transport
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Lecture - 29
Nanoscale Energy Transport in a Thin Film Part 3

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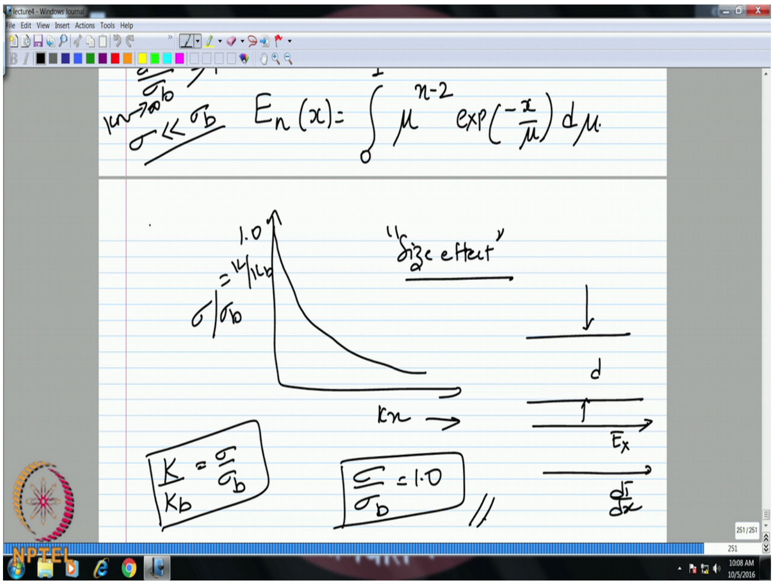

I think some of you may might, still not have completely gone through run over the derivation that we did yesterday. Let me quickly summarize once again. So, the important thing when we talk about Nanoscale Energy Transport is to first understand you know whether you have a transport parallel or perpendicular if you consider a particular nano structure.

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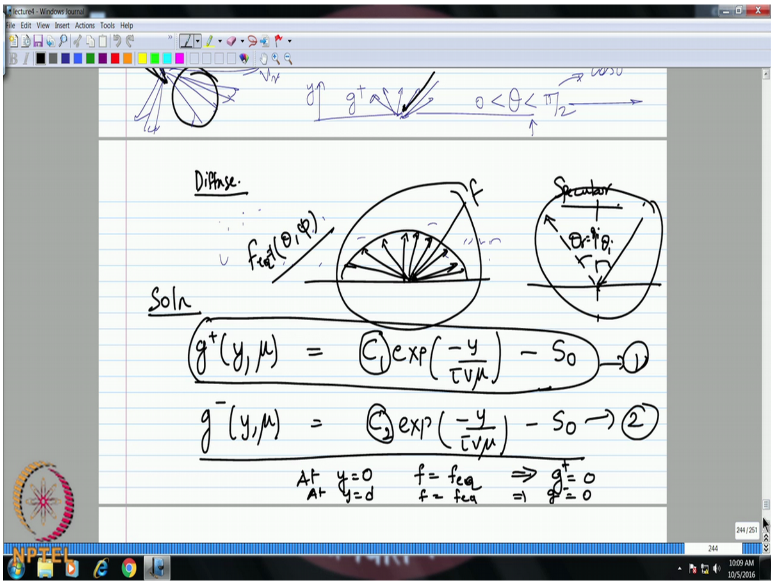

So, depending on that, so, you have to formulate the Boltzmann transport equation and for the case of electron transport which contributes to current flow, so that is the example I have considered and I have also taken case of transport of electrons along the x direction and the confinement of the film along the perpendicular direction. So, for such a case we have written down the Boltzmann transport equation which is of this particular form.

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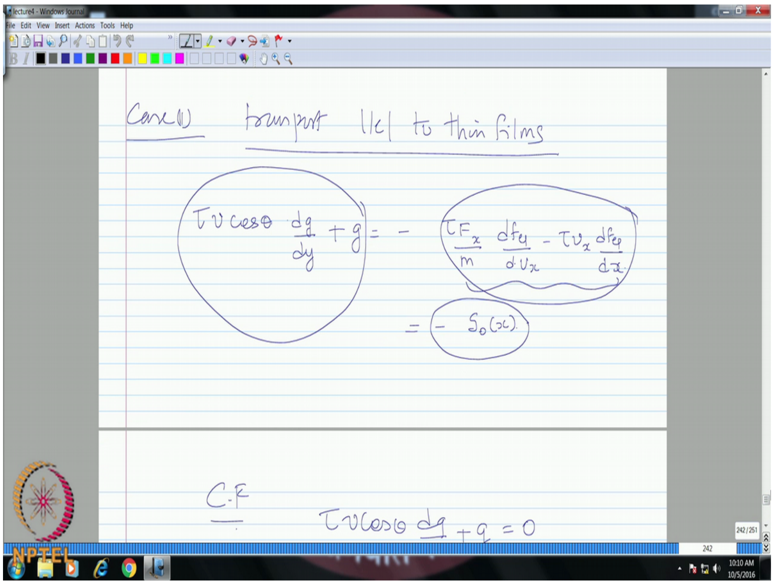

And what is important here is to find out the (Refer Time: 01:46) function g and its variation with respect to y. So, this is what is going to result in the size effects. So, therefore, now we have an ordinary differential equation which we could solve and then we could get a solution in terms of you know y and s naught of x right.

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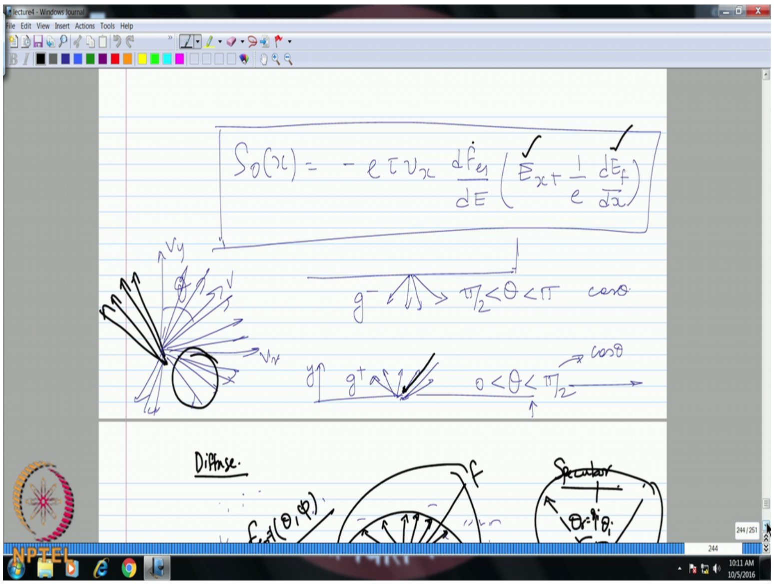

Where s naught of x for the case of electron charged transport is you know given by this particular expression.

Now, after this point is now coming to the solution. So, we have 2 contributions to this butter patient function or any non equilibrium distribution function because this non equilibrium distribution function is now going to have a directional dependence. So, therefore, it is going to vary with theta even in case of 1 dimension. So, it will have a variation with respect to the direction cosine cos theta.

In this case we have to split up the distribution function into 2 components 1 which is going in the positive y direction the other going negative y. So, we have identified those 2 components. So, that we can apply the 2 boundary conditions at y equal to 0 and y equal to d and find out the constants. So, accordingly we determine the complete solution.

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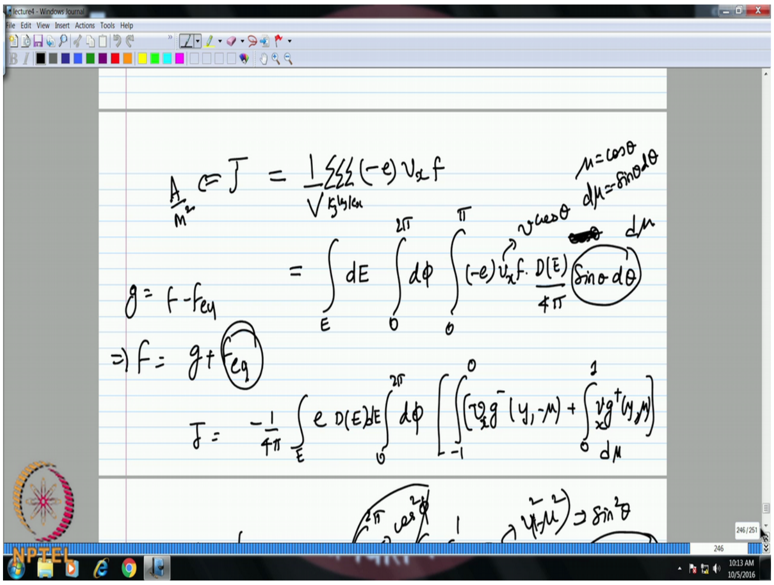

So, this is what you get g plus and g minus. Once you get the distribution function. So, all that is required now is to put this in the expression for the charge flux or the current flux. So, therefore, in terms of F if you write. Basically, we know that F is equal to g plus F equilibrium and then if you integrate F equilibrium over the solid angle it is going to be

0 because this uniform not varying around mean about the solid angle and integral cos theta sine theta d theta will be 0.

So therefore, all we are having this we end up with an expression only in terms of g plus and g minus. So, we have split the polar angle or you know from 0 to pi by two and pi by 2 and pi by 2 to pi. So, we have written that in terms of the direction cosines. So, correspondingly minus 1 to 0, 0 to 1.

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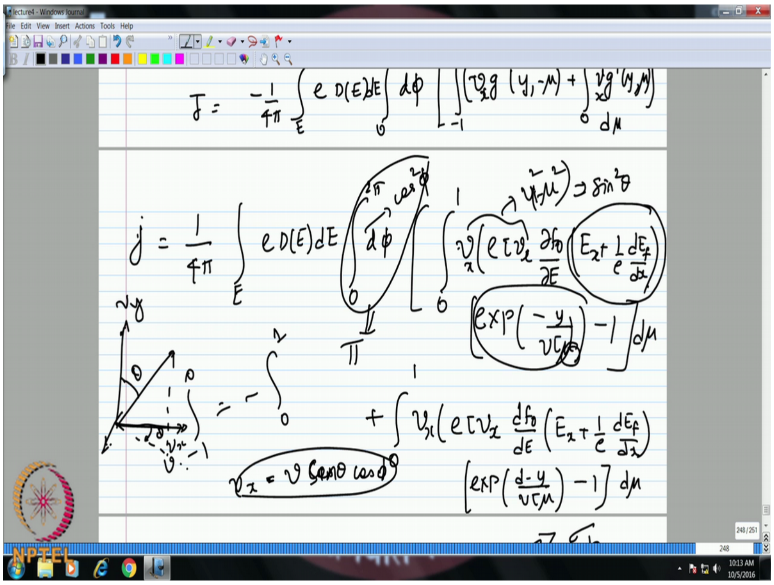

And then, in the expression for g no we already have this v tau mu. So, in the case of negative direction cosines minus 1 to 0 we can write this basically as you know value of mu here is going to be negative and we can replace this from 0 to 1 and the corresponding value of mu will take negative values. Whereas, if you look at the other side it is going to be positive. So, that is how we have rewritten this in terms of mu and replaced the limits from 0 to o1ne instead of minus 1 to 0 and then after this is simply integration you know.

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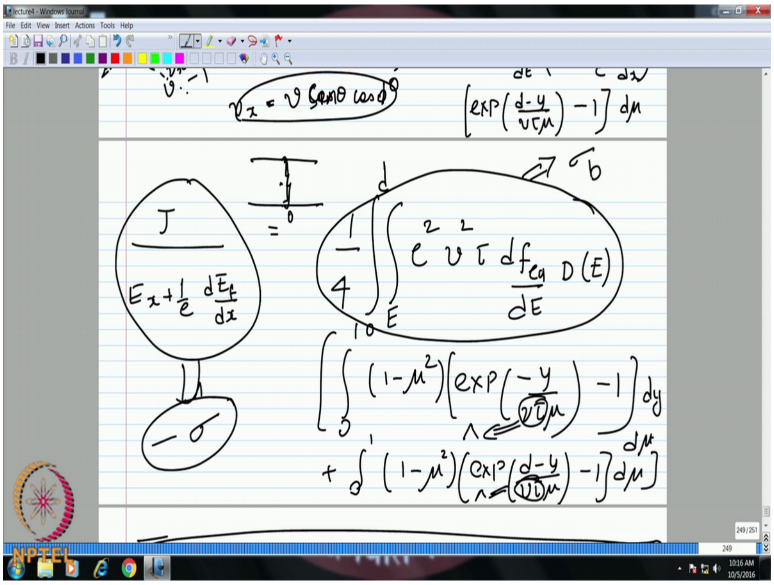

So, we do use all the rules of integration and finally, we write the terms on the left hand side such a way that we have current flux divided by the electric field plus whatever the electro chemical gradients.

So, this is equal to basically you electrical conductive right and on the right hand side we have basically a more complex expression out of which we can identify this group of terms here, which is a circled basically is nothing, but similar to your bulk electrical conductivity and 1 more thing I just I forgot yesterday is that you know this is a flux correct so; that means, if you are talking about transport between 2 plates if you are talking about some point you are evaluating this quantity. Similarly if you want to calculate the total flow just like heat flux and heat flow.

So, you have current flux and current flow you have to integrate this over the entire length from 0 to d. Therefore, we have to also do 1 more integration here from 0 to d Dy. Because we also have a variable y here in the solution for g, g is a function for y therefore, to also when you finally, get the solution you want a net quantity we do not want a electrical conductivity which is varying with y that does not make much sense although I mean it is a flux and also it is a function of y, but finally, when you are talking about thermal conductivity electrical conductivity they are for the entire system.

Therefore, what we need to do is integrate this expression across that particular plane from 0 to d Dy and; however, we are dealing with on the left hand side terms of flux. So, the right hand side now it is in terms of the integral values therefore, we have to divide by d in order to still make it a flux unit. So, that is the only thing I think I missed yesterday and if you do this integral with respect to y.

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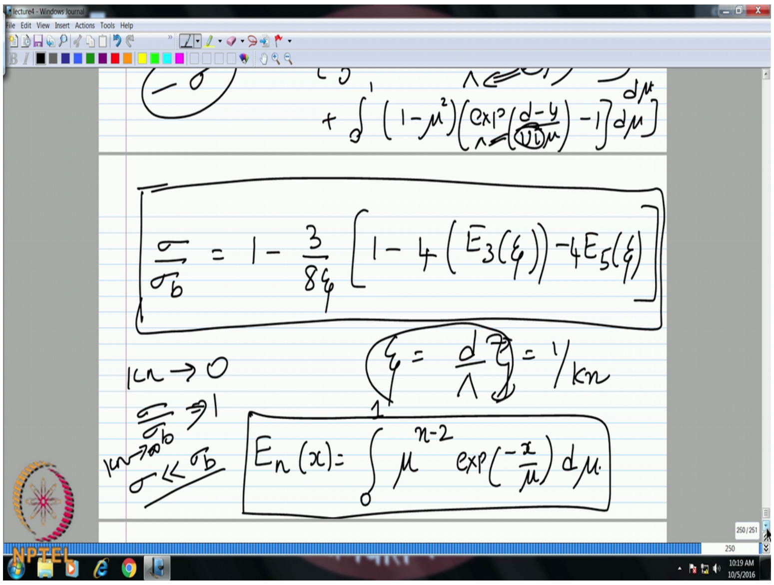

And also with respect to mu you have 2 integrals double integral we have terms 1 minus mu square exponential minus y by v tau can be replaced with the mean free path time's mu. So, therefore, this entire expression is a function of variables mu and y you have to integrate them and if you integrate. So, you can with respect to y if you first integrate. So, all the y is will be replaced with d. So, then you will be simply having a non dimensional parameter d by lambda which is yes. So, this is your zeta which is your 1 over Knudsen number right. So, inverse of your Knudsen number apart form that you have to now integrate with respect to mu. So, those integrals I have expressed in terms of the integral functions E 3 and E 5. So, you have 2 terms here. So, 1 if you multiply this quantity with this you have you have 1 parameter mu times exponential of this right.

So, when you first integrate with respect to y you get this mu parameter and then next other parameter will be there will be mu cube times this. So, there are 2 integral functions. So, that is why I denote them as E 3 and E 5 where it evaluate the corresponding E 3 and E 5 integral using this expression. We finally reach this point which gives you the ratio of electrical conductivity for any Nanoscale film as a function of your bulk electrical conductivity.

So, what it means is if your Knudsen number is very small your zeta value goes to infinity and this term minus that 2nd term will disappear and therefore, it will reach the bulk value and for larger values of Knudsen number your electrical conductivity is reduced right. So, same way if you work out an expression for the thermal conductivity whether it is thermal conductivity or only electrons or you take case of phonons you will also get a similar expression similar to the ratio sigma by sigma b you will get k by k b which is similar to that.

So, I think this is what we have seen.

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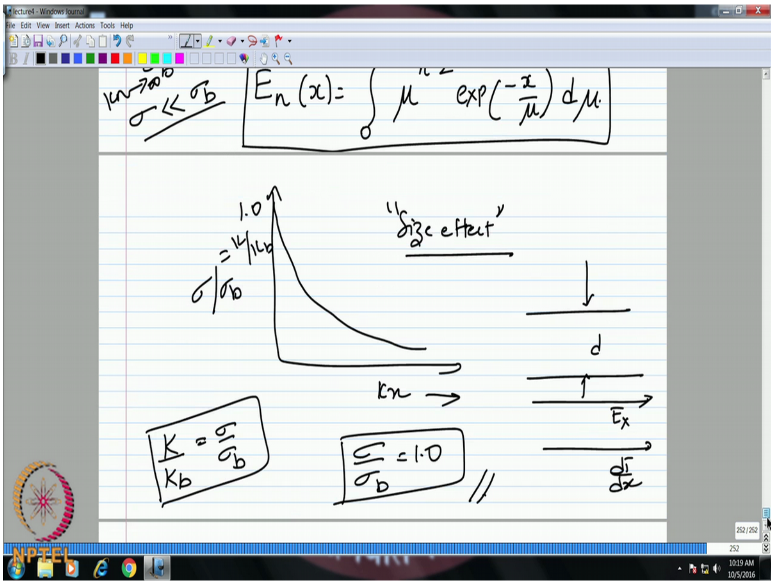

So, I mean all you have to is you have to go home and make sure you work out again and the steps intermediate steps. So, then you become more comfortable with derivations that are it is not difficult. So, we have already done most of this before. So, only that you have to be careful with the integration.

Student: (Refer Time: 10:57) negative only that the (Refer Time: 11:00) when we take the ratio negative side will be continuity that angle to integration.

You are talking about the mu.

Student: No.

Negative in the.

Student: No (Refer Time: 11:10) zeta minus 1 upon (Refer Time: 11:13) these 2 j and j minus (Refer Time: 11:16) then minus 1 is comes to the equation divided sigma we get bulk.

Student: Then that time also will be.

You are saying that the sigma b is having a negative sign is it.

Student: Minus e square integration of something.

Minus e square is it. So, what do we have here do we have a minus e square.

Student: So, the negative negative sign will be cancelled.

In that case we have to retain you may be right because I think we have negative sign here because this 0 to 1 is basically absorbed here. So, already we put a negative sign. Therefore, there is no reason that this should simply disappear yeah. So, you may be right. So, this will continue till here and.

Student: (Refer Time: 11:59).

Correct. So, we can just say that this is your including your negative sign this is your sigma b right. Yes I think you can be, but at least if you are not careful with the signs in a negative sign you know on for the entire term then it is, but inside the within the terms you have sub terms. So, if you make mistakes then you will have wrong expressions.

Yes, because these are all very lengthy expressions. So, it is very difficult to keep track of you know all the signs 1 after the other possibly 1 of the length lengthiest expression in this course right. So, this is the case for transport parallel to the films and also with diffused boundary conditions diffused catering of the boundaries what happens when you have specular scattering at the boundaries.

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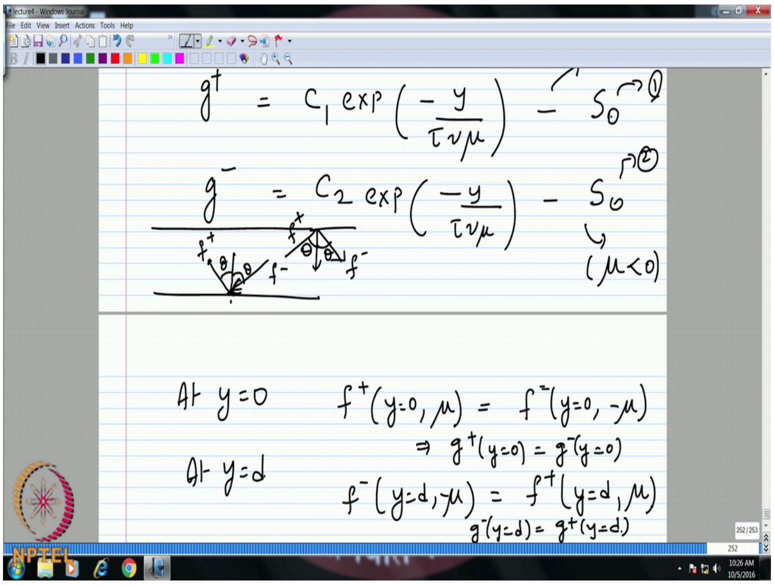

The solution general solution in terms of C1 and C2 is still going to remain the same that is not going to change only you have to apply the specular boundary conditions to determine the constants. Therefore, your g plus will be C1 still the same expressions that we had written down minus s naught g minus will be C2 minus s naught. So, this for the case where mu is greater than 0 this is for the case where mu is less than 0 this direction cosine positive and this is downward direction.

Now, all that we have to do is what specify the boundary condition for speculars scattering. So, at y equal to 0 if you are talking about specular surface, so you have an electron or phonon which is coming in a particular direction theta and it is going to scatter with the same angle the other direction. Similarly, on the top boundary also incident and reflected angles are the same. Therefore, at y equal to 0 you are if you call this as f plus right that is the distribution which is scattered going in the positive mu and this is your f plus or f minus this is coming into the boundary f minus this is coming with the negative direction cosine into the boundary and that gets scattered and its coming out in the positive direction.

So therefore, at y equal to 0 what is unknown is f plus because that is what is coming out of the boundary. So, therefore, in this case f plus at y equal to 0 comma mu will be equal to f minus at y equal to 0 comma minus mu right. So, whatever distribution function is incoming is just reflected without altering the value of the distribution, but only the direction is changed in the sense that it is a mirror image of this. So, it is coming in the know negative mu and now this is giving in the positive mu, but with the same angle the same direction cosine and same magnitude this is like a mirror image.

Similarly, at y equal to d. So, at y equal to d what is need to be determine f plus or f minus. This 1 what is coming out of the boundary f minus what is reflected f plus. So, therefore, f minus at y equal to d comma minus mu is equal to f plus y equal to d comma mu correct. So, also this means f equilibrium is independent of direction the same thing can be said about g plus. So, g plus at y equal to 0 is equal to g minus at y equal to 0 and similarly at y equal to d is equal to g plus y equal to d. So, therefore, you please use these 2 conditions into these expressions determine the constants C1 and C2.

Student: (Refer Time: 17:56).

Yes, just I have given that, but you do not have to. So, as long as you know that f minus corresponds to negative mean you do not have to put a negative sign. So, you please substitute this find out the constants. What you get?

Student: (Refer Time: 20:04) first condition (Refer Time: 20:06).

So, from first condition y equal to 0; so you get c one equal to c 2, but still that does not tell.

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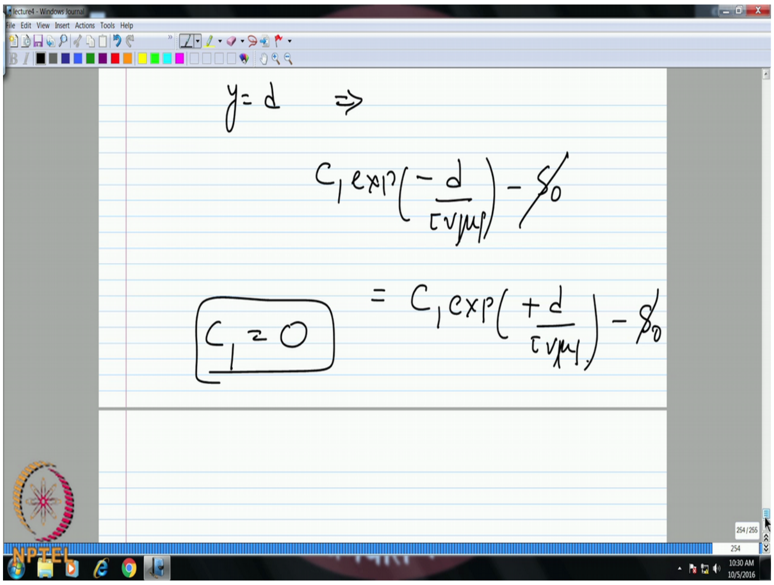

What is the value of C 1? So, then you have to apply the 2nd condition y equal to d. So, that is telling you C1 is exponential minus d by tau v mu minus s naught equal to C1 exponential minus d by tau v mu minus s naught. So, s naught s naught cancels even this also will cancel yeah because here you have to be careful this mu is negative. So, if you want to properly you know write it you can put magnitude of mu and this is negative if you put magnitude of mu then this will be positive, that is may be a clearer way of explicit way of writing.

Now, what we are saying now this expression left hand side should be equal to right hand side, but clearly how can this be possible you have one side positive mu another side negative mu. This can be equal only if C1 equal to 0. So therefore, C1 equal to C2 equal to 0. Then what happens to g plus and g minus they becomes same right. So, g plus equal to g minus will be equal to minus s naught.

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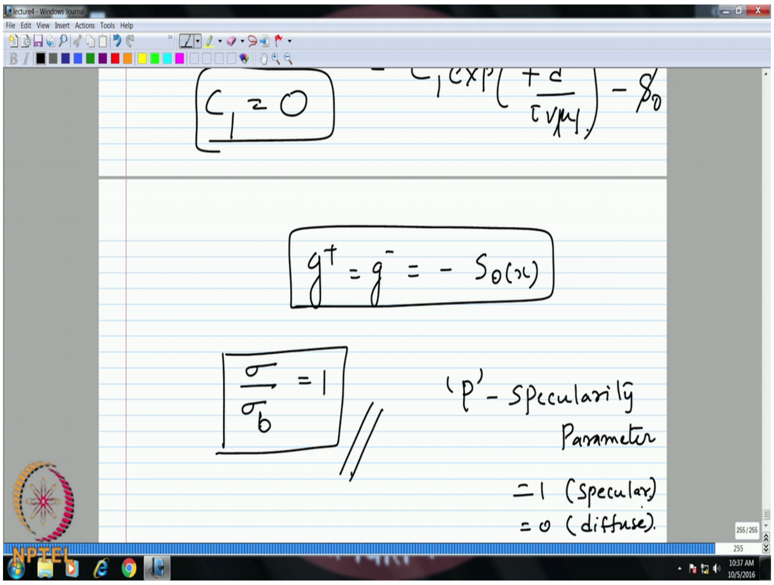

So, now you go back to the expression for charge flux and substitute this and see what happens.

Student: Sir (Refer Time: 22:57) g minus (Refer Time: 23:02) as d minus y function.

No the d minus y function comes from the diffused boundary condition correct, for the specular case now we are starting from again the general solutions the d minus y comes because the diffused boundary condition your constant turns out to be exponential d by tau v mu your f is equal to f equilibrium. Please go back and see what we have done yesterday this is the condition we get what diffuse. So, the constant C2 turns out to be that. So, you can complete that exercise I will only give you the final result. So, this will simply come out to be this.

Student: (Refer Time: 25:58).

Correct.

Student: (Refer Time: 26:04) both are same.

Both are same. So therefore, the other additional terms that 1 by 3 minus sigma d that will actually not come right. So, all these integral functions with respect to mu and all will not be there. So, only you have the sigma b term on the right hand side. So, it very simply turns out to be the same as your bulk electrical conductivity. So, this is now completely different expression you know just if you change the boundary condition you see that there is no modification in your electrical conductivity for this case. So, therefore, the nature of the boundary condition tells you whether there will be a distraction in momentum or not in the case of specular boundary condition you are perfectly observing the momentum.

So, whatever is incoming distribution is same as outgoing because there is no loss of momentum and therefore, there is no need for reduction in the conductivity or electrical or thermal whereas, in the case of diffused scattering there is an associated reduction in the energy of the emitted phonon or electron due to this distribution over the entire (Refer Time: 27:32) polar angles. So, that will result in consequent reduction in the conductivities. So, therefore, it is very important to understand that you cannot simply say electron transport parallel to film is always resulting in reduction depends on kind of boundary scattering that you are applying.

Most of the real time surfaces are neither entirely diffused nor entirely specular. So, they will be somewhat in between. Therefore, how do we categorize that we use what is called as a specularity parameter. So, this is given by notation p and if this is equal to 1 it indicates it is a purely specular scattering, if it is equal to 0 it is completely diffused most of the real surfaces are between 0 and 1 we do not know exactly, but it can vary from 0 to 1 and depending on whether you have a specular or diffused parameters we have independently got the expressions now what happens when you have somewhere between 0 and 1.

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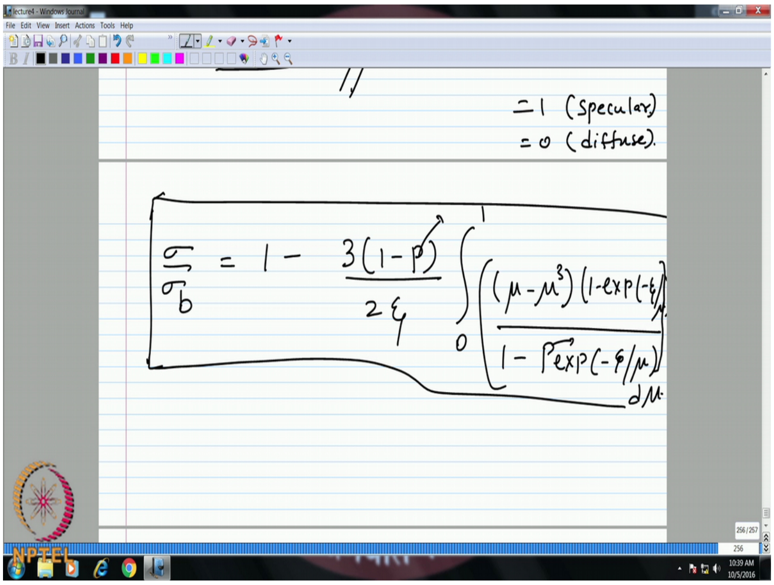

In that case the expression turns out to be including this specularity parameter also. So, you have the splecularity parameter p appearing these cases when you put for example, p equal to on1e this entire term disappears and you get your other expression if p equals to 0 you get back your diffused scattering expression. So, this is also very generic case for different values of specularity parameters.

Student: (Refer Time: 29:58).

Yes, that is the yes. So, that is the integral. So, 0 to 1 entire expression times d mu you have to integrate it I have not explicitly written the integral functions now. So, as e 3 5 I have just given the total expression. So, the last part that I want to I do not want to derive this because this is somewhat clumsier than the transport parallel to the film and might confuse you. So, what I will do is the case where transport is perpendicular to the film I will only give you the final expression and anyway since you are going to do this programming assignment.

So, you will be doing the programming assignment for the transport perpendicular to the film you can also do parallel to the film and compare with this expression you can give either diffuse or specular and you can verify whether you are getting similar to this analytical solution, but mainly the more challenging case is the transport perpendicular to the film. So, you will solve the Boltzmann transport equation and find the numerical solution and I will only give you the analytical solution with which you can compare with your results.

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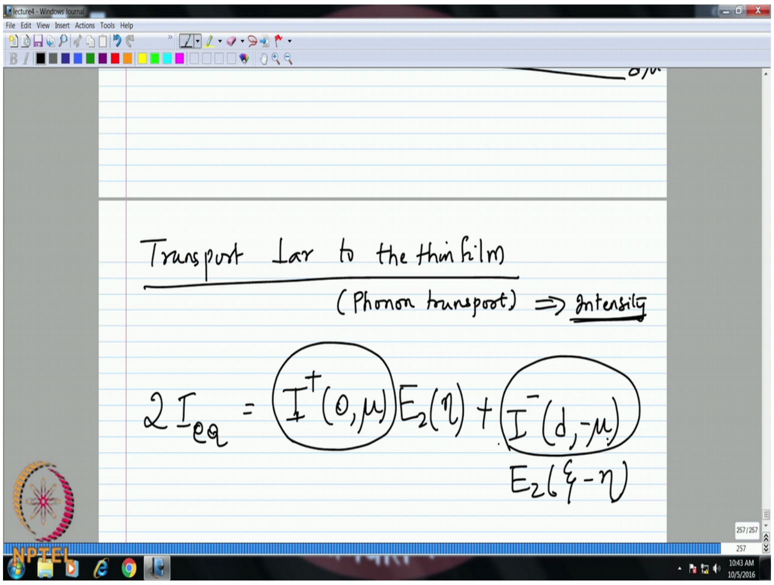

Therefore, for the case where you have transport perpendicular to the thin film; so if you go back and revisit what you have derived the Boltzmann transport equation for the transport perpendicular to the film.

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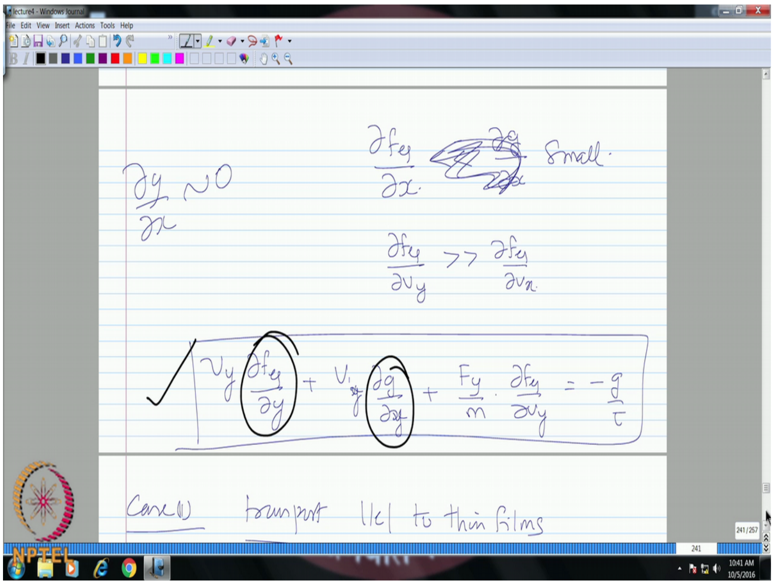

So, this is the expression correct. So, we have both f equilibrium as well as g both of them in the direction where the transport is. So, now, if you solve this I will give you the final expression I will write the final expression in terms of the intensity for example, right now what I will do is I will only give you the expression for phonon transport because that is what you are going to do in the numerical solution also phonon transport and I am going to express distribution function in terms of intensity.

I have also uploaded the reference paper on noodle, which gives you the equation cast in terms of the intensity of phonon transport. So, you will be solving in terms of rather than distribution function intensity it is just a small multiplication nothing more. So, therefore, because y intensity is much easier as you can directly get the expression for temperature from intensity similar to a radiation. So, in radiation also you define the total intensity from which you directly extract your temperature.

In a similar way when you are talking about phonon transport we are interested in finally, plotting the temperature distribution. So, if you are calculating the distribution functions then you have to convert that in terms of equivalent temperatures and then get that also can be possible, but more elegant way is to write directly the Boltzmann transport in terms of intensity and therefore, your temperature can be directly extracted. So, in terms of intensity the solution, this is your equilibrium intensity here in place of f I am just writing in terms of I 0 mu and again these are integral functions the same integral functions what I have given for the parallel case should apply here also. This is I plus at y equal to 0. So, basically the boundary condition what you are applying at y equal to 0 is this particular intensity and at y equal to d that is your boundary condition I minus intensity of the phonon which is coming out at y equal to d in the downward direction.

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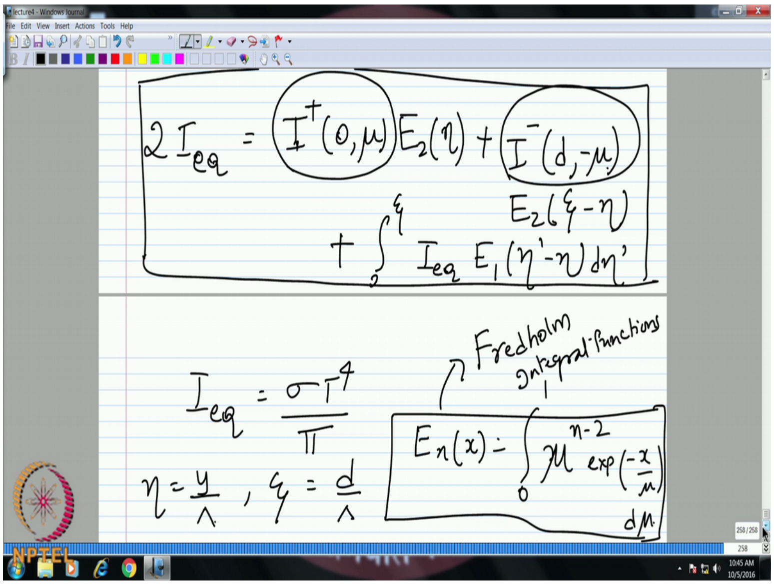

So, this plus; so you have 3 terms essentially 0 to zeta I equilibrium E1 eta prime minus eta d prime eta prime is a dummy variable. Where, now I equilibrium is related to your temperature like this and your integral functions mu power yeah u power n minus 2 exponential of minus x by mu d mu the same integral function. These are popularly called as Fredholm integral functions. So, all we have you have to do is calculate the temperature distribution as a function of eta.

So, eta is nothing but your non dimensional y. So, I am defining eta as y by mean free path and zeta is nothing, but inverse of your Knudsen number. So, this expression if you plug in solve it in met lab or even excel sheet this will give you the temperature as a function of y or non dimensional eta 0 to whatever values. So therefore, this is the expression now if you plot it how the temperature distribution looks.

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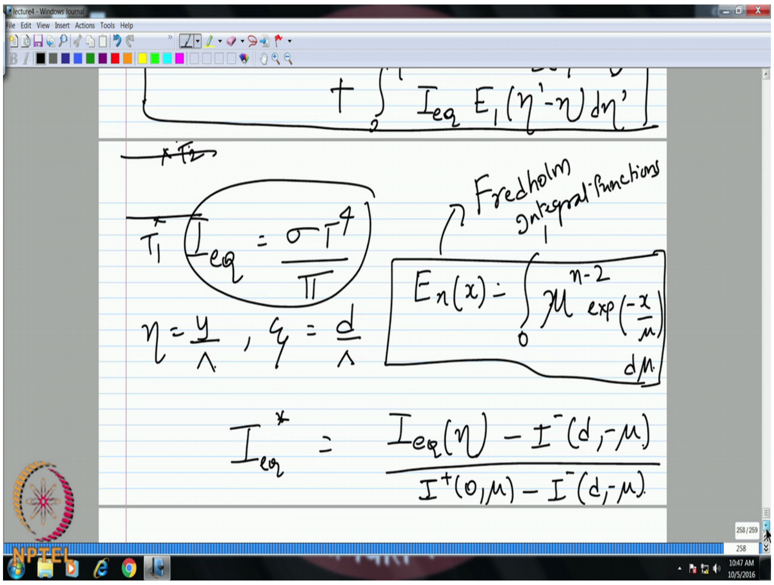

So, I would like to define a non dimensional intensity I will call this as I equilibrium star which is a kind of non dimensional temperature because we have related the equilibrium intensity with temperature right. So, it is similar to plotting your non dimensional temperature right. So, this is defined as I equilibrium eta that is basically this expression as a function of eta minus this is your boundary condition at y equal to d right and the boundary condition at y equal to 0 minus the boundary condition of intensity at y equal to d.

So, I am basically non-dimensionalizing my local temperature with the boundary temperatures. So, this value of I plus and I minus can be calculated from the corresponding boundary temperatures. So, if I fix my bottom boundary condition at T1 and T2 I can use this expression calculate for T1 what is the value of I equilibrium at the bottom wall and similarly for T2 what is I equilibrium on top wall and therefore, whatever is coming out should come out with that particular intensity right. So, that is dictated by the boundary conditions or temperature boundary conditions at the top and bottom; so if I normalize and plot, so the normalized temperature versus eta.

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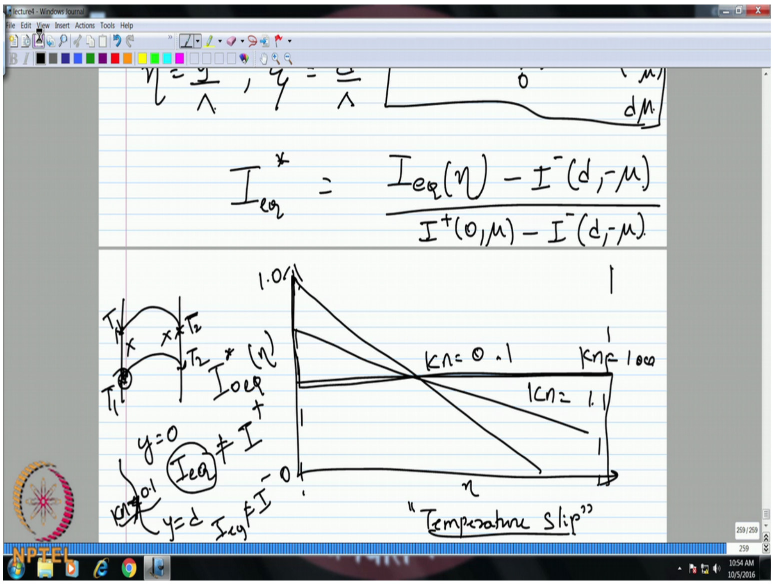

So, that is the local variation of temperature with position. So, this value will be between 0 and 1 right it cannot exceed the boundary value, at Knudsen number of point 1 what will you expect? This is similar to here furriers law a linear variation in temperature from one end to the other now as your Knudsen number keeps increasing this could be Knudsen number of 1 suppose you go put a very high Knudsen number Knudsen number of 100 for example,. So, in that case get a perfectly flat line. So, what does this indicate?

Student: (Refer Time: 40:30).

So, there are no scattering between phonons. So, for very large nook sun numbers approaching infinity this is called ballistic transport right. So, hardly the phonons see each other. So, the directly the phonon from this boundary will come and hit this boundary. So, this is at temperature T1 this is at T2. So, it will come with an intensity corresponding to that temperature and directly land on the 2nd surface, but what happens there is a shock because the second surface is at temperature T2 and this phonon does not know that. So, therefore, there will be a discontinuity at the boundaries.

So, this is your boundary right these are your boundaries. So, this phonon will see a shock here and the similarly the phonon which is going from this to this. So, it is having temperature T2 here it lands on this boundary, but it finds that temperature is T1, but it cannot now adjust already it is gone and it is stuck there and therefore, you find there is a jump. So, these kinds of discontinuities at the boundary or temperature jumps are characteristic of this nanoscale transport.

At macro scale you will never have that because the phonon collusions are sufficiently so much so that they can transfer all the information from 1 end to the other, but in the nanoscale sub continue on regime this transfer is not possible because you do not have complete information communication between energy carriers. So, you end up with all this discontinuities or in other words if you look at y equal to 0 there you are, I equilibrium will not be same as what is the emitted phonon intensity understand. So, the emitted phonon intensity will be different from the corresponding equilibrium value. The corresponding equilibrium value equilibrium means it is an average or you know summation of the phonon intensity in all the directions.

So, what is coming out will definitely be different be from what is coming in. Therefore, you are I plus will not be same as I equilibrium and what is I equilibrium that is the indicator of temperature temperature now how do we define in nanoscale there is no it is not a physical equilibrium thermodynamic temperature in nanoscale. So, temperature here is only an indicator of local energy. So, local energy density you have to somehow express this and therefore, we call this as temperature, but and fortunately this becomes the same value as the physical temperature in macro scale. Therefore, it is more appropriate to refer this in terms of intensities or energies rather than in terms of temperature and similarly.

So, at y equal to d your I equilibrium is not the same as your I minus, if this was there then what will happen this is the case where you nook sun number is less than point 1 then this will be equivalent to your fouriers law. So, everything has it at local equilibrium. So therefore, there is no temperature jump, but for a case where you know Knudsen number greater than your point 1 we are talking about say ten or 100 or 1 in all these cases these is not satisfied. So, this is a very important characteristic. So, people also refer to this as temperature slip, this kind of temperature discontinuity as temperature slip right. So, this is the characteristic of transport perpendicular to the film.

So, I think we will stop our discussion on nanoscale energy transport with this because more or less you have enough idea what is happening even in 1 dimension. So, so the basic the key understanding is that you know all the size effects are becoming very important at higher Knudsen number. So, when we talk about now temperature distribution this is this is basically temperature slip correspondingly a thermal connectivity also will start reducing because of this. So, these are additional resistances at the boundaries. So therefore, effectively your nanoscale thermal connectivity will be lower and this keeps dropping with increasing Knudsen numbers.

So, from tomorrow's class we will start looking at micro scale and transport micro scale will appear much easier. Now that we have done the nanoscale because we have the proper foundation, so also the equations are more familiar to you. So, most of them are continue equations. I hope that you know most of you were able to follow at least 70 or 80 percent of this content. Sometimes it might be completely new altogether, new topic, and we have it is also intensive mathematically, but nevertheless it will give you a new perceptive about this kind of transport.

Thank you.