Micro and Nanoscale Energy Transport
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Lecture -28
Nanoscale Energy Transport in a Thin Film Part 2

Film was attempted by him in 1993, those are Arun Majumdar and in the case that the distribution function there is not explicitly used. But he defines the moment of this distribution function called intensity. And based on this intensity he solves the Boltzmann Transport Equation in terms of the intensity of what he calls is Phonon Radiative Transport. So, he coins a name called E P R T Equation for Phonon Radiative Transport, it is nothing but the same Boltzmann Transport Equation the relaxation time approximation and cast in terms of intensity of phonon transport a phonon radiation. So, that is return in terms of f equilibrium.

So, I mean he uses a numerical technique and he solves this is one dimension, use a simple finite difference is ok finite difference should give you a solution, but what is important is we have seen this distribution functions are not only function of physical position just one dimension it is not just function of x, but also function of, for example, polar angle theta. So, you have to also solve this in theta space. So, you have to therefore, numerically discretize you are physical space as well as your spherical coordinate space physical space meaning your x here, and also the directional space which is your in terms of theta.

So, you have to discretize this into discreet number of directions between theta going from 0 to pi and phi going from 0 to 2 pi phi it is going to be uniform in terms of phi that is the assumption of one dimensional transport and then use the finite difference method and solve this numerically.

So, integration can be done by using trapezoidal rule or any stranded numerical techniques Simpsons rule that should workout and if you take high number of grid points. So, if you discretize it in a very fine manner you will be able to accurately match it with the analytical solution.

So, I want to you to write this programme to do that the reference is the paper by Professor Arun Majumdar 1993, I thing it appeared in journal of applied physics. If I remember. So, the title is something like equation for phonon radiative transport and it talks about basically writing the b t in terms of intensity solving that numerically and getting the solution for different Knudsen Numbers s from Knudsen Numbers s of 0.001 all the way up to Knudsen Numbers of 100 where it is a ballistic transport. So, you simply get a big discontinuity at the boundaries and then you have a horizontal line. So, we have looked at that kind of solution before. So, he talks about all this.

So, I want you to write this programme all by yourself. So, you can use what are programming language you would like whether it is a proton or c c plus plus or matlab python whatever you want to use. So, it is a not that difficult it is only basically 2 dimensions one physical coordinate the other is the directional coordinate. So, you should discretize them use some method to calculate the integrals and therefore, solve it for temperatures and plot the temperature distribution as a function of Knudsen Numbers s. So, by that you will understand exactly whatever we have done, I am giving you some analytical solution. So, how do you actually solve the b t for more complex cases then you will be able to know the procedure and compare it with this kind of simple solutions all right.

So, today and tomorrow let us work on the remaining part of this transport equation try to find some simple solutions before we go on to the micro scale part. Therefore, we started off from the b t again you have made some approximations and again, we have derived to sets of t t is, one for the case where transport is parallel to the film and for that case we saw the f equilibrium is in the direction where the transport happens in the case where you have coordinate system where the transport is happening in this direction, the equilibrium distribution varies in that direction. Whereas if you look at the (Refer Tim: 05:46) from the equilibrium. So, this is the indicator of the non equilibrium.

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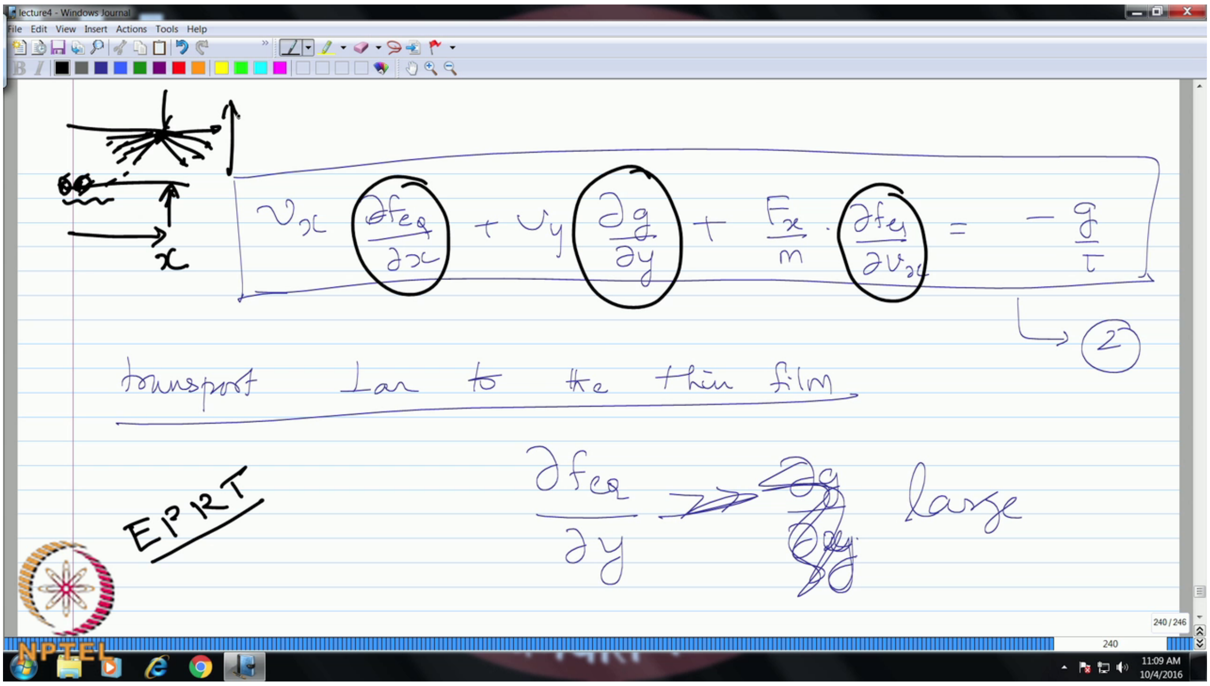

So, this non equilibrium if it also happens along x, there is no size effect because the film is confined in this direction perpendicular to the transport direction. Therefore, in order to bring the effect of this dimension on to transport the deviation from equilibrium should vary as a function of y and not as a function of x the reason is that; now as we know if, you take at this particular point. So, you have the phonons which are basically scattered from all directions right and falling on to this point and similarly they are scattered out. So, there is phonons which are coming to this particular boundary and they are scattered by the boundary.

So, as you see that these are direction dependent and each of these phonon if you physically track the coordinate each of this will actually come from different points along x right. So, they will be originating physically from this point and then, they propagate in that direction and they reach this boundary similarly from another position another set of phonons in a different direction will rich the same point on the boundary.

Therefore, you see that this, phonons are carrying information which as which are now basically showing a variation along x. So, that goes and scatters and therefore, why dj y dj by dy contains the information of the confinement is this. So, basically you have there is a change in the equilibrium distribution function along x and now, since it is also direction dependent.

So, this information is conveyed to during this scattering of the phonon from the boundaries and therefore, there is a gradient now set up in also the vertical direction for the deviation from the equilibrium. So, dj by dy. Now will start vary right along y also. So, this is now going to carry all what we call as size effects similarly the transport perpendicular to the film is quite straight forward. So, you have transport in this direction therefore, equilibrium function varies in that direction and also the deviation from equilibrium will also be dominant in only the y direction because of the confinement.

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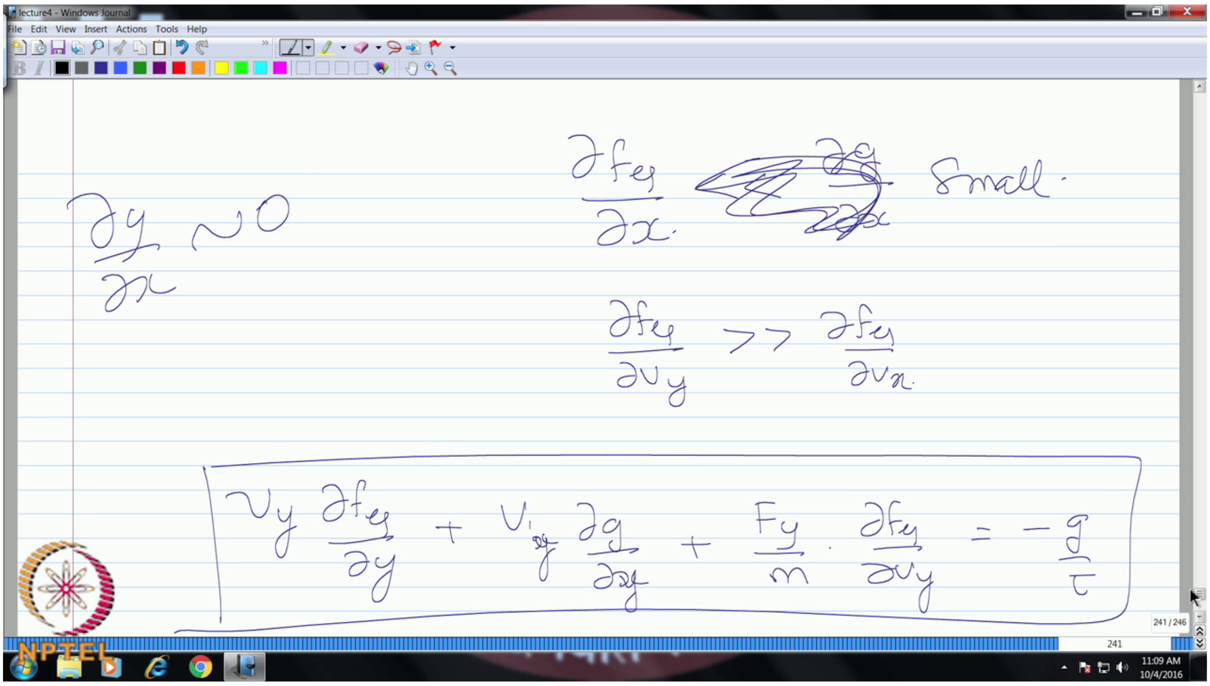

Therefore for that you have only all the derivatives with respect to y. Therefore, we first started with the transport parallel to the film we separated out the terms which are functions of y, these are the most important terms that is we have to solve for g basically and all the terms with respect to f equilibrium we retail on the left hand right because, these are the functions which are known f equilibrium is known which ever distribution function you take and you can therefore, find out the derivative with respect to x and v x, whereas, what we need to know is solve for g which gives you the non equilibrium distribution.

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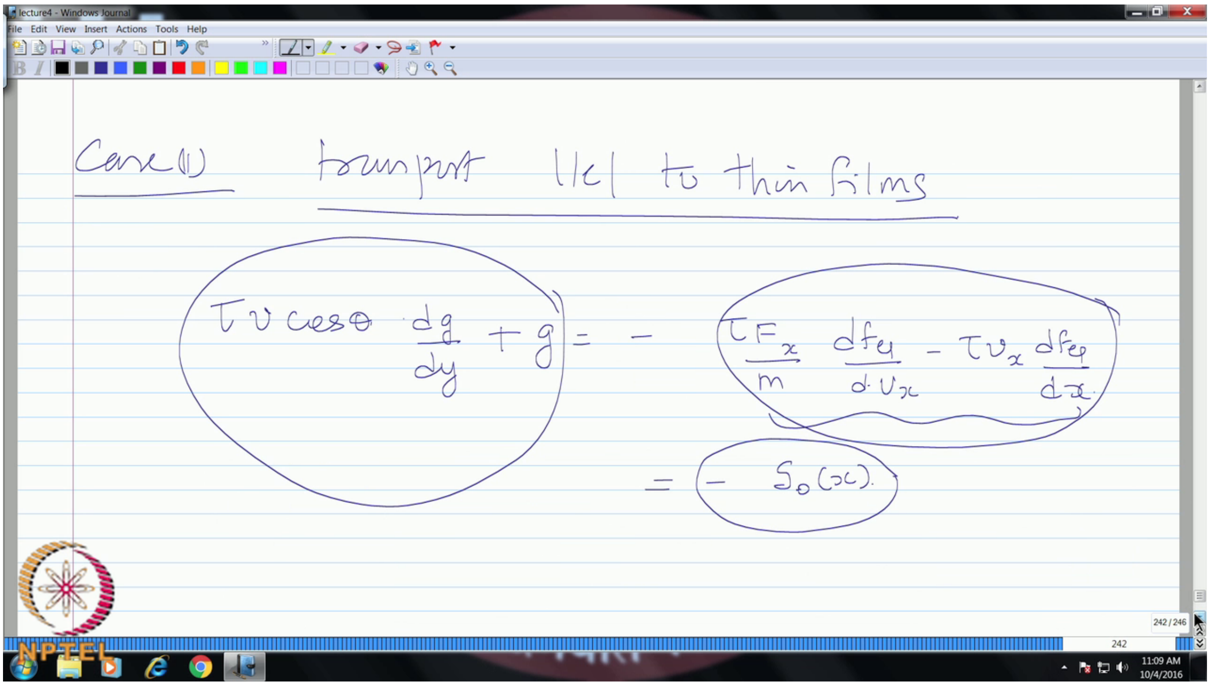

Therefore, S naught of x can be now written for example, in the case of charge transport it comes out to this particular form.

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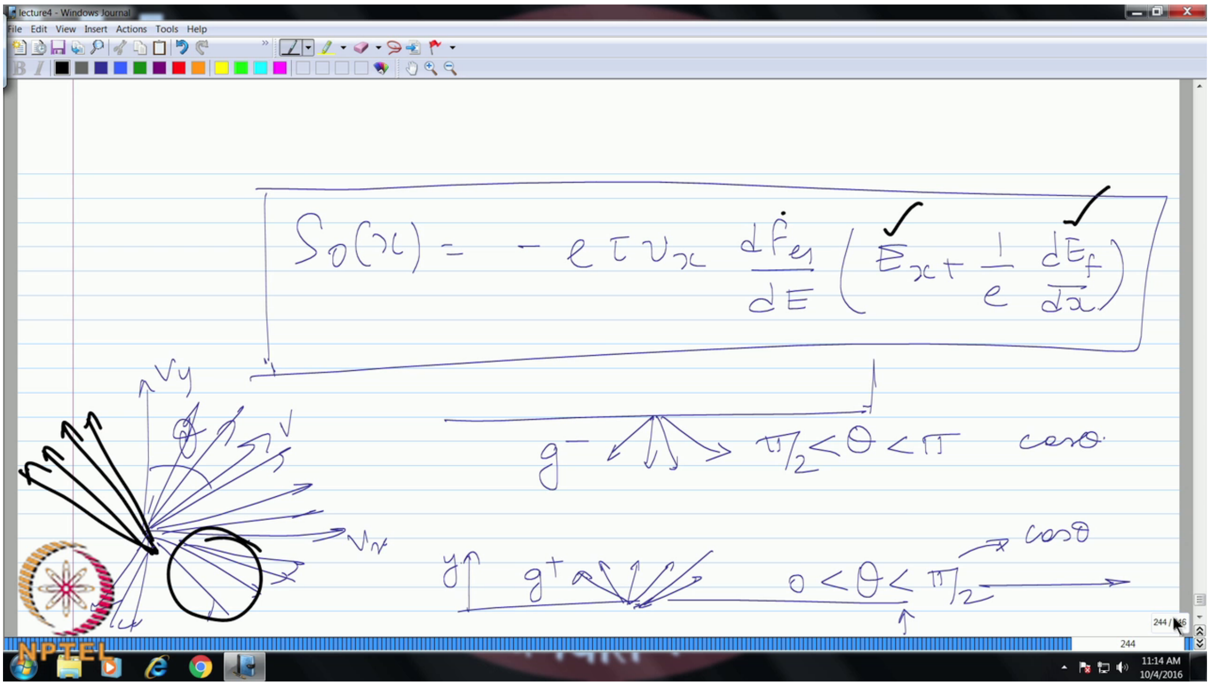

So, the variation of f equilibrium with respect to x is coming from the dependence of the Fermi level on x that is this term and the other term is the variation with respect to v x in the momentum coming from in the variation of e on that. Therefore, we have 2 terms 1,1 with the respect to the variation with respect to the momentum the other with respect to the physical space is that clear.

Therefore, this will be your term which is the function of x and which is known; if we know d e d e f by d x you just simply substitute it the electric field you can substitute it the variation of d v equilibrium d f equilibrium by d e.

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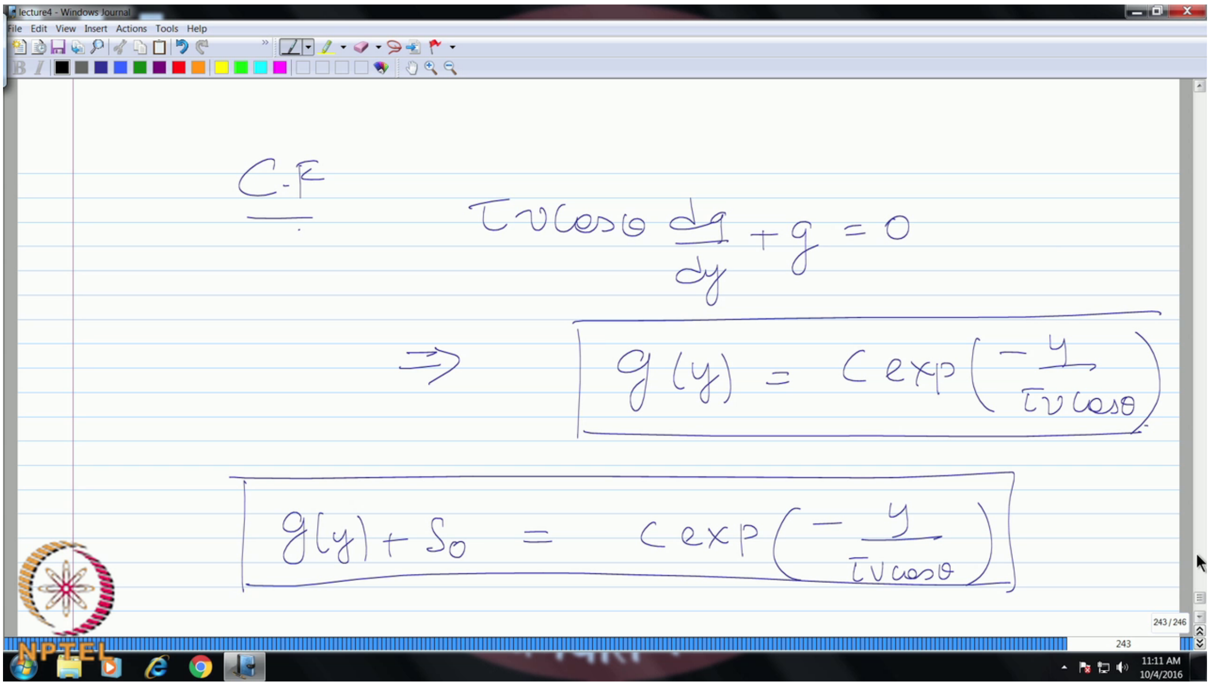

So, now what we can do is solve for g which gives you the non equilibrium distribution function. So, so as we as we saw that we if you solve for g the full solution become g of y plus S naught is equal to this, now this is the function. Therefore, g is not only a function of y, but also function of theta. So, it is carrying therefore, both the directional coordinate as well as the physical coordinate. So, if you want to break this down into the transport of electrons going in the positive y direction and the negative y direction.

Therefore, if you look at the top boundary for example, the top boundary is going to scatter whatever electrons come to that boundary are going in the negative y direction. Therefore, the direction cosine for this will be negative. So, the theta in that case will be varying from pi by 2 to pi. So, the pi by 2 to pi will contain information of all these scattered phonons in the down ward direction and similarly the phonons reaching the bottom boundary will have phonons scattered 2 in the positive y direction.

So, there the theta will vary from 0 to pi by 2 and the direction cosines will be positive right. Therefore, at every point we can break this g into a positive g and negative g because we have only transport in the y direction. So, which are going in the positive y and scattered scattering the negative y.

So, we can actually divide therefore, this g into g plus and g minus right and therefore, I hope you could can follow till this point right and your Azimuthal angel phi is varying from 0 to 2 pi. So, that makes thus distribution symmetric. If you are solving from theta 0 to pi by 0 and then, you are rotating from phi 0 to 0 pi. So, you are going to get the same distribution with respect to theta in the other side also. Therefore, we do not have to really bother about what is happening to the distribution on this side on this side this distribution is going to be just simply similar to this your theta your phi is going to rotate this and make it make it a symmetric distribution about the vertical access, I hope you understand this. Therefore, the most important directional coordinate will only be theta there will be only a variation with respect to theta and not with the respect to phi.

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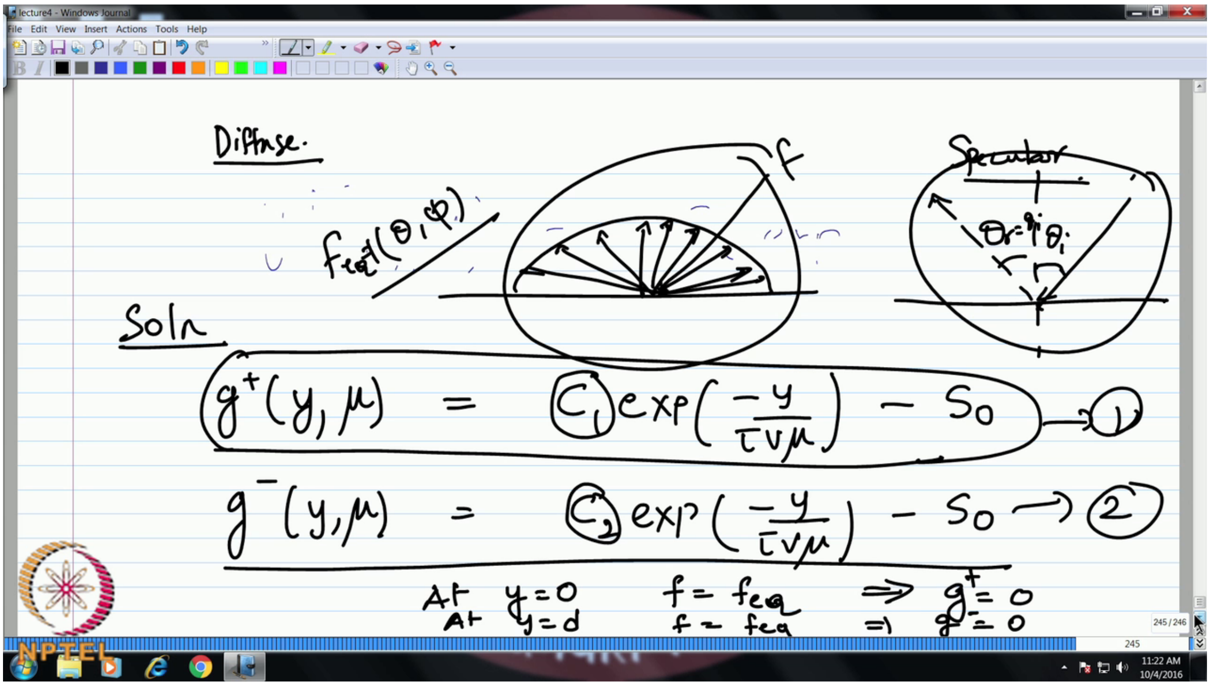

Now, knowing this, we can have 0 solutions. Therefore, the solution can be written as you have a g plus which is a function of y and the directional cousin mu in which is nothing, but cos theta that is the cousin which it makes with the respect to vertical assess right we have theta with the respect subtended with the respect to the vertical accesses. So, that will be your directional cousin.

And in the general solution we had a constant. So, we will write this as C1exponential minus y by tau into v into mu I am writing my cos theta as mu minus S naught and similarly my g minus will be another constant C0 this constant is going to be different from this because this corresponds to the distribution going in the positive y and therefore, I give a plus sign. So, this constant is going to be different for this scattering going in the downward direction, but the other terms will remain to be similar. So, why we are writing this in terms of 0 functions is actually one function. But we have identified a positive y and negative y is to apply the 0 boundary conditions because, we have scattering from the top wall scattering from the bottom wall. So, they are going in certain direction from the top it is going down from the bottom it is going up.

Therefore, it is convenient to break this in to 0 distribution functions at every point to find out the constants using the 0 boundary conditions. So, if you apply the boundary condition at y equal to 0. So, what kind of boundary condition can we apply now, that is the next important question? So, the one that I have described here is the case were you have a particular phonon or electron which is coming in the direction like this. For example, and this is getting scattered in, many different directions, there are 0 extreme cases of scattering. So, one is called diffuse scattering. In this case now you can imagine this boundary to be quite rough. So, any incoming electron or phonon will get uniformly scattered with the same magnitude in all the directions. So, you can draw a length of these arrows uniformly to represent they are all of the same magnitude.

So, this is quite similar to your radiation transport in radiation also you have a particular intensity of incoming wave which hits the boundary and can get scattered or reflected. So, we have 0 different kinds of reflections one is a diffuse reflection were the intensity of the reflected beam is uniform the same magnitude and uniformly spread over all the directions this is similar to the diffuse scattering we are talking here the other is specular you can imagine the surface to be very smooth like mirror finish and therefore, if a particular electron or phonon comes and makes an angle theta I this is your incident angle. So, it gets reflected such a way that theta r is equal to theta I and it gets reflected only in the same direction.

Therefore, this is completely different kind of a boundary condition compare to this. So, in other words this is a kind of a boundary condition where, any non equilibrium distribution function if it encounters a diffuse interface or diffuse boundary will get converted into a equilibrium distribution function which is uniform because a what is the characteristic of equilibrium distribution function it is? It is uniform with the respect to directional space there is no variation only you have a variation with respect to the physical coordinate, but not with respect to directional space. So, when you say f equilibrium f equilibrium is not a function of theta and phi.

Therefore, whenever your phonon distribution function encounters the diffuse interface your non equilibrium distribution f will become equal to f equilibrium because, it is uniformly scattered whereas, in the case of specular it is not? Therefore, to apply the boundary condition at y equal to 0 at that is at the bottom surface our f will now become equal to f equilibrium in the case of diffuse scattering and therefore, this will tell that g will be equal to 0. So, these are 0 extreme cases the real surface will be combination of both of them. So, similarly at y equal to let us say d this is at the top boundary again your f will be equal to f equilibrium and therefore, g will be equal to 0.

So, now when we are saying this g here what does it indicate g plus or g minus the first one at y equal to 0 g plus and here g minus. So, we can therefore, put this in the corresponding distribution at y equal to 0. So, we will be using let me call this as 1 and this is 2. So, at y equal to 0 will be using 1.

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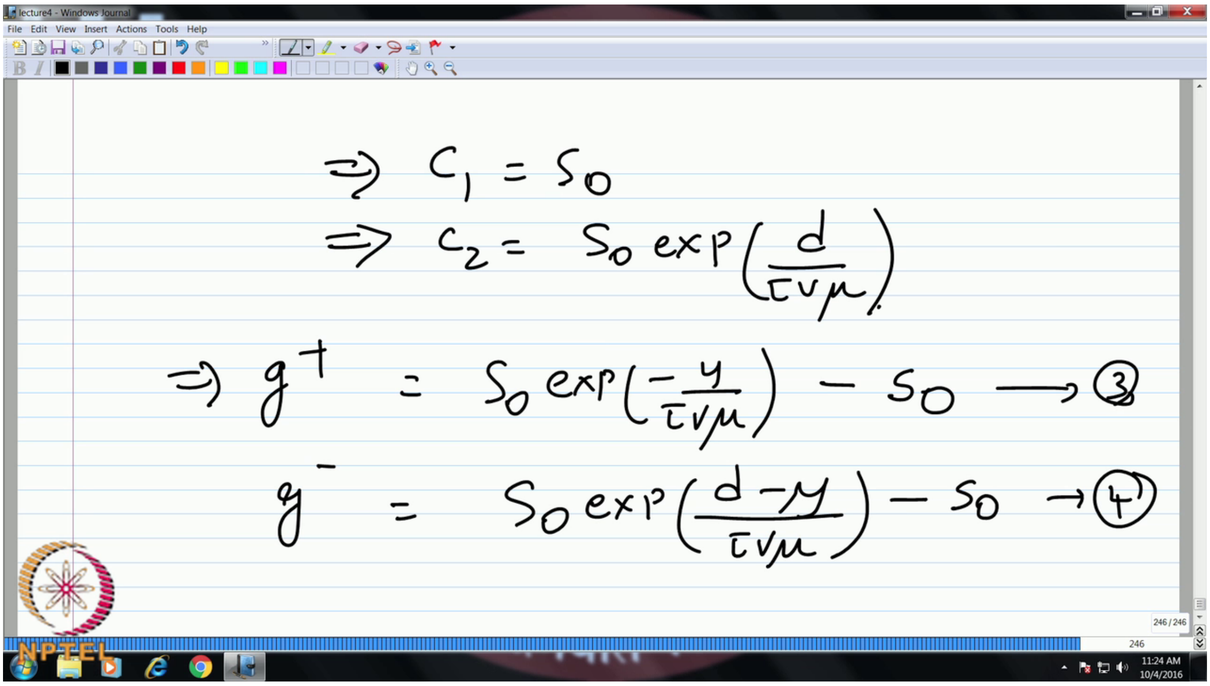

So, can you substitute and let me know what is the constant C1 S naught. So, you have C1 is equal to S naught from the second boundary condition your C0 turns out to be S naught e rise to d upon tau v mu.

Therefore if you substitute this in terms of g plus will become S naught into exponential minus y by tau v mu minus S naught and we have g minus which will be S naught exponential d minus y by tau v mu minus S naught will call this as equation 3 and 4. Is that clear? There substituted for C1 and C0 that is it.

Now, now that we know the non equilibrium distribution functions in the positive y and negative y, all we need to put calculate what is the flux of the charge, how do we do that we already know how to do this right. So, let us call what is the notation we used for charge flux.

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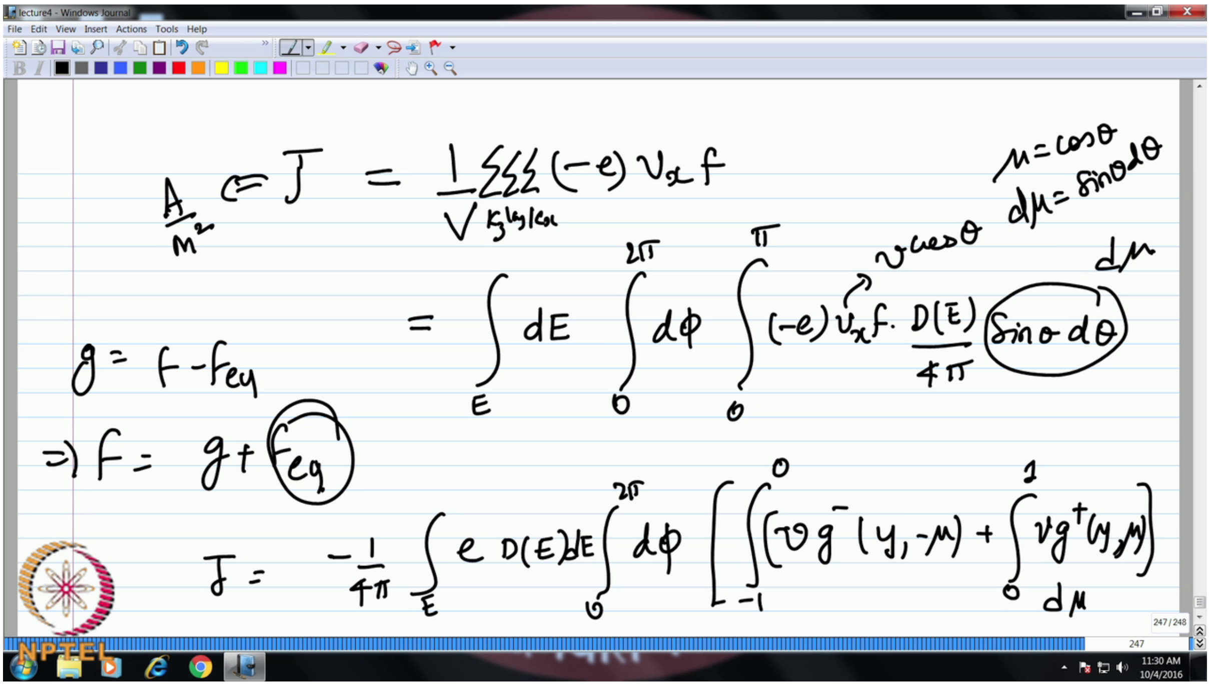

Student: j

J we used j. So, let us use the same. So, j which is indicating your charge flux or current flux, how do we calculate it? Do you remember from your distribution function? You should not even go back you should just by now know how to do it. So, for a single quantum state what is the charge flux.

Student: (Refer Time: 23:55)

Minus e v x into f per unit volume. Now, therefore, integrate over all the quantum states k x k y k z. So, this will give you ampere per meter square. So, if you convert this now how to convert the summation into integral dkx, dky, dkz from which, you can use density of states covert this momentum space into coordinates involving theta and phi correct. So, what do you get in terms of theta and phi.

So, we have one integral over d e and then 0 to 0 pi d phi and then, we have 0 to pi minus e into v of x f we have density of states d of e by 4 pi sin theta d theta v of x is nothing, but v cos theta is that clear we already did this conversion before while deriving the continuum equations. Now, all we are doing going to do is what we know solution for g which is nothing, but f equilibrium minus f. So, we define g as f minus f f equilibrium or f equilibrium minus f I think, it was f minus f equilibrium, right? f minus f equilibrium f minus f equilibrium and therefore, we can write f as g plus f equilibrium we know the solution for g from equations three and four all you have to do is break this 0 to pi from 0 to pi by 0 and pi by 0 to pi.

So, that is positive direction cosine and negative direction cosine. So, write in terms of g plus g minus. Therefore, now j will become minus one by 4 pi e d of e this is over energy and then we have 0 to 0 pi, it is not varying with the phi space. So, this can be taken out. Now with respect to 0 to pi, my cos theta is nothing, but mu right mu is equal to cos theta therefore, d mu will be sin theta d theta. So, I can write this as d mu and this as mu and therefore, my limits of integration will become, if I put cos 0 mu will be 1 cos pi will be minus 1. So, it will be minus 1 to 1. So, I can break this minus 1 to 1.

Student: (Refer Time: 28:00).

Yeah. So, minus one to 0 v of x or v times g plus g minus here minus one to 0 indicates the negative cosine. So, will use g minus y comma minus mu this indicates negative one plus 0 to one v g plus y comma mu all this d mu right into this is de. Therefore, all we can do is sub now what happen to f equilibrium integral f equilibrium cos theta sin theta d theta d phi 0 because f equilibrium is a uniform in theta and phi direction. Therefore, if you integrate cos theta sin theta d theta d phi is going to be 0.

So, now you can substitute for the solution for g plus and g minus. So, if you do that I will only give you and also for S naught. So, S naught we can substitute from here. So, if you do that.

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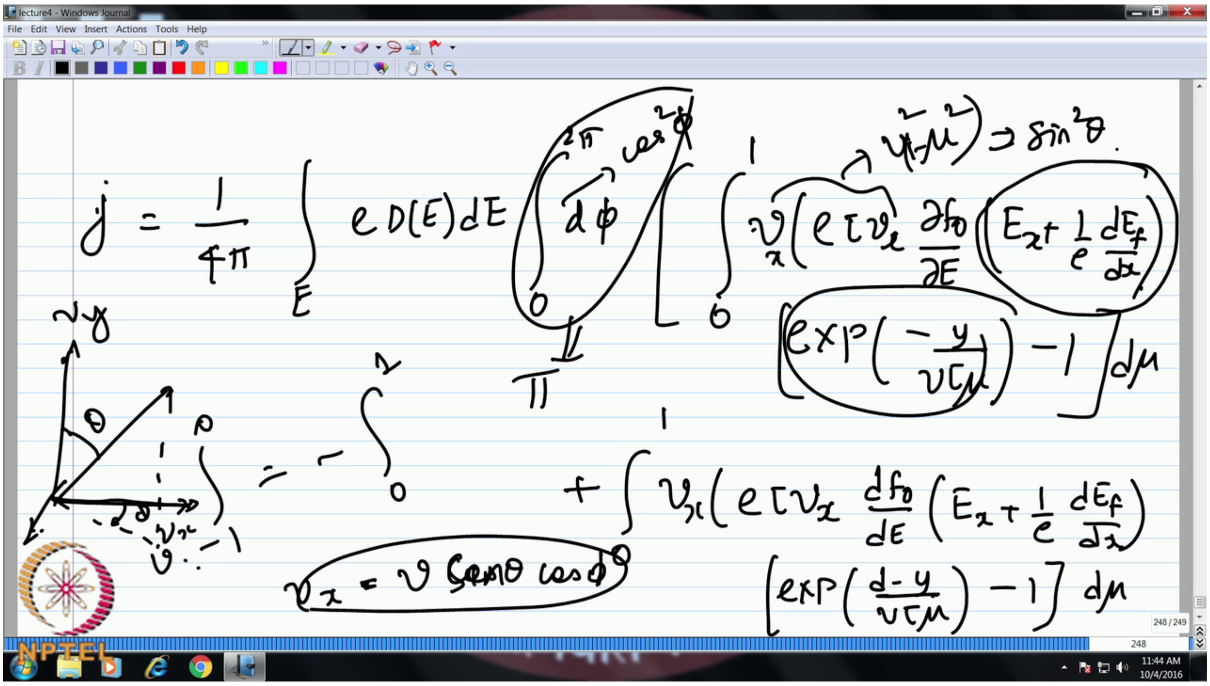

So, you will get a lengthy expression j one by four pi get e e d of e d e 0 to 0 pi d phi and 0 to 1 v into e tau v x b f naught by I am substituting for S S naught here into e x plus 1 by e d e f by d x exponential minus y by tau minus 1 d mu essentially equation 3 I am taking S naught common. So, we have this minus 1 and S naught have simply substituted from there.

So, this is on one half the other half will be 0 to 1; we have v into e tau v x d f naught by d e into e x plus 1 by e d e f again S naught and exponential we have d minus y by v tau mu minus 1d mu. So, I have one v x here. So, that should become b square let me see did I miss.

Student: cos theta

There should have been a cos theta again extra right I think yeah so.

Student: (Refer Time: 33:02) mu e.

Yeah, but I think this v x should be there, but there should have been a extra cos theta there right. So, in the d omega that is your solid angle should be cos theta sin theta d theta d phi correct. Therefore, there should have been the additional cos theta, am I right? Therefore, we can right this just thing in term of v x here and just simply continue.

Student: (Refer Time: 33:42)

Yeah. So, that cos theta is mu.

Student: (Refer Time: 33:46)

So, v x I am just living it as it is. So, v x is going to be just v cos theta I will observe it in the next step. So, there is again one more v x where we will again have a v cos theta. So, will have cos per theta there. So, we have v x v x coming here and then. Therefore, we will have v x here v x here. So, we have v x square which is v square cos per theta.

So, that is nothing but v square again mu square. So, we can also write in terms of that. So, can you now rewrite this in term of mu and try to find out what will happen if you integrate with the respect to mu? So, you have this function is a function of mu and your v x square is nothing, but v square.

Student: Mu square.

Mu square.

Student: (Refer Time: 35:08)

Yeah. So, I we can write minus 1 to 0 as equivalent to minus of 0 to 1 mu

Student: and also gives negative sign the mu

Yeah. So, that I think that I am this have been observed when I got a positive sign here.

Student: (Refer Time: 35:24)

I do not think so.

Student: (Refer Time: 35:27)

There will be 3 negative signs here.

Student: (Refer Time: 35:33)

Yeah minus sin theta yeah I think, but you are right this will be again minus sin theta d theta, but I think finally, what I work out is you get only a positive sign here, we have to check that again please we have to be careful here just hold down v x is not cos theta here it is sin theta because our notation is this is my theta and this is my v x . Therefore, v x will be v sin theta. Therefore, this will be 1 minus mu square this nothing, but sin square theta.

Student: (Refer Time: 36:33)

Ha.

Student: v y is v cos to.

Yeah v y is v cos to theta. So, in this case we have taken theta to make to be angle with the vertical and our transport is in the x direction. So, that will v sin theta and therefore, you will have 1 minus mu square this sin call theta. So, please integrate it with respective mu I think.

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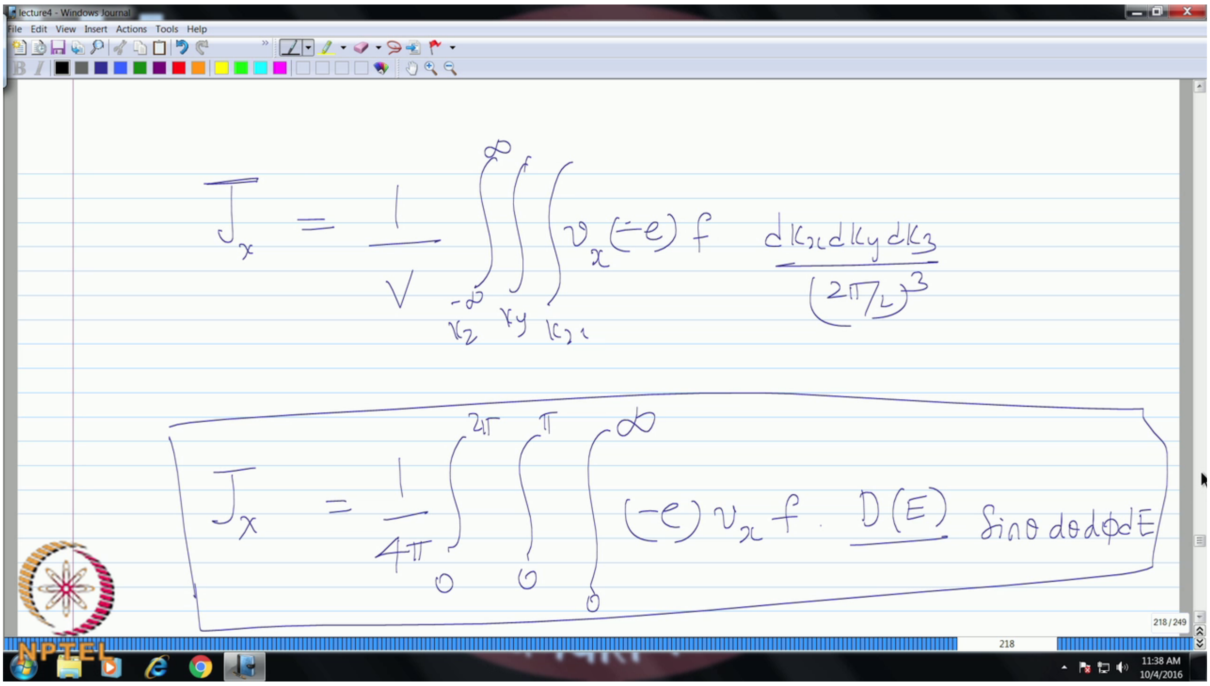

Student: mu cos theta

Mu will be.

Student: sin theta.

Mu will be cos theta here mu in the sense now that is the positive y and negative y. So, that will be with the respect to cos theta we have v x still I am not completely convinced about my think this is. So, I think few more thinks now. So, will we write v x it should it should be just a second. Yeah. So, let me again clarify this your v x is not simply v cos theta it is v cos theta. It should be v sin theta cos phi because in a 3 d you are looking at this projection in this particular plane which is making an angle phi. So, you have to actually look at v cos phi which is basically this one and your also looking at this cosine in this direction. Therefore, it is v cos phi sin theta right. So, that is your direction cosine in the x for this case.

Therefore, you also have a cos phi. So, there will be a cos square phi also in addition to this. So, will be adding cos square phi to this d phi and this. So, this d mu now I think now I mean this d mu is fine. So, we do not have to therefore, do anything here I think all things are falling in place. So, you have to be careful that we are working with transforming theta to mu. Therefore, our sin theta d theta is become the mu and again when we are talking about transport v x here. So, that is nothing, but v sin theta cos phi.

Therefore, we have v square sin square theta cos square phi and sin square theta we can write as 1 minus mu square and cos square theta you have as integral 0 to 0 phi cos square phi d phi. So, to just give you, this integral 0 to 0 phi cos square phi d phi will be equal to pi you can evaluate and check this and finally, So, you should. So, you have a common term. Therefore, see a therefore, we can take this entire term e x plus 1 by e d e f by d x out and therefore, we can write this as j and you can bring this to the denominator.

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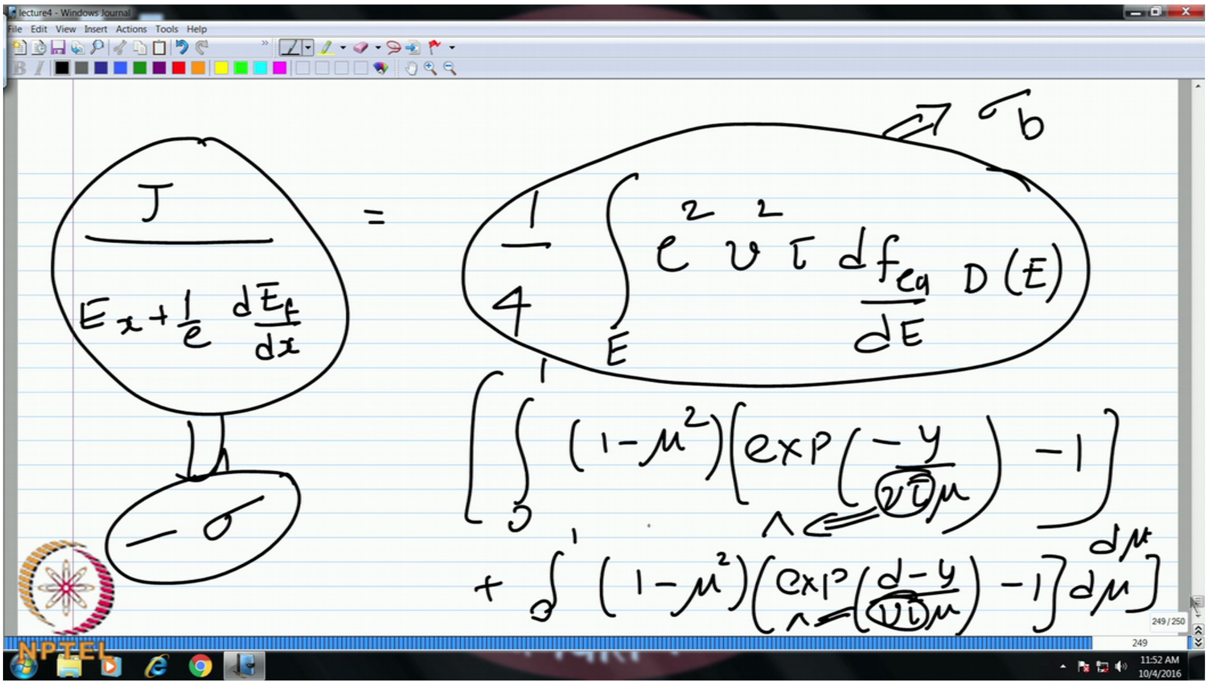

So, we have e x plus 1 by e d e f by d x. So, this will be equal to 1 by 4 and we have over e we have e square v square tau and we have the dependence on e will be through d f equilibrium by d e we have d of e. We have very lengthy expression here. Therefore, we have there is an e here and e here. So, we have e square and we have v square d f naught by d e d xf d e.

So, this is the term common term e f e of x plus 1 by e d e f by d x is taken out and to the other side. So, we have this term here and the others are all dependent on mu. So, we have 0 to 1, 1 minus mu square into exponential minus y by v tau mu minus 1 d mu plus 0 to 1, 1 minus mu square exponential d minus y by v tau mu minus 1 d mu. So, this pi cancels because our integral cos square phi d phi is phi. So, this 1 by 4 pi and that pi cancels of right. Now please go back to our derivation of ohm's law what was the expression for electrical conductivity that we got? Which term is it?

Student: (Refer Time: 46:10)

Now, therefore, if you look at it apart from that apart from that we also have these additional terms which are nothing, but the size effect terms. So, now, if you look at j divided by e x plus 1 by d e f by d x what is this what is your homes law say your j should be equal to electrical conductivity times your electric fail e of x plus f if you have a electro chemical potential 1 by e d e f by d x right. Therefore, this entire term here is nothing, but minus sigma you understand. So, when you divide this current flux by the electric filed this is nothing, but minus of sigma. So, j should be minus sigma of this. Therefore, this is minus sigma. Therefore, the expression for electrical conductivity, now where he have Nanoscale transport is equal to this and out of which we obtain that the bulk value of electrical conductivity expression is this correct.

I hope all of you are able to follow. So, the expression for bulk value that we have derived let us go back to that this is your expression we have minus e square integral tau v square d f equilibrium by de d of ed e we have minus e square by 3. Therefore, we can write this as we can multiply and divide by 4 ok.

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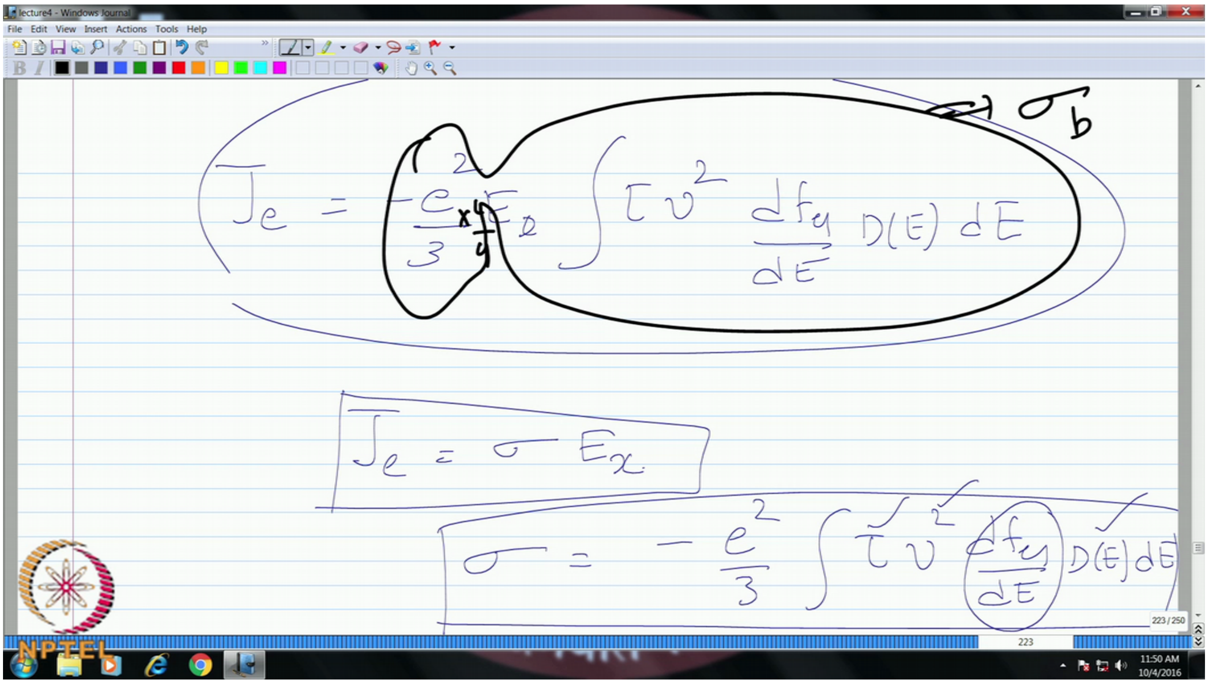

Therefore, what we have here can be rewritten in terms of the bulk thermal conductivity. So, this entire term is nothing, but your bulk electrical conductivity understands. So, j e by e x is nothing, but a bulk electrical conductivity.

If you therefore, write this in terms of sigma by sigma b, the expression on the left is nothing, but sigma and what we have is in terms of sigma b therefore, we can write directly an expression for ratio of sigma by sigma b.

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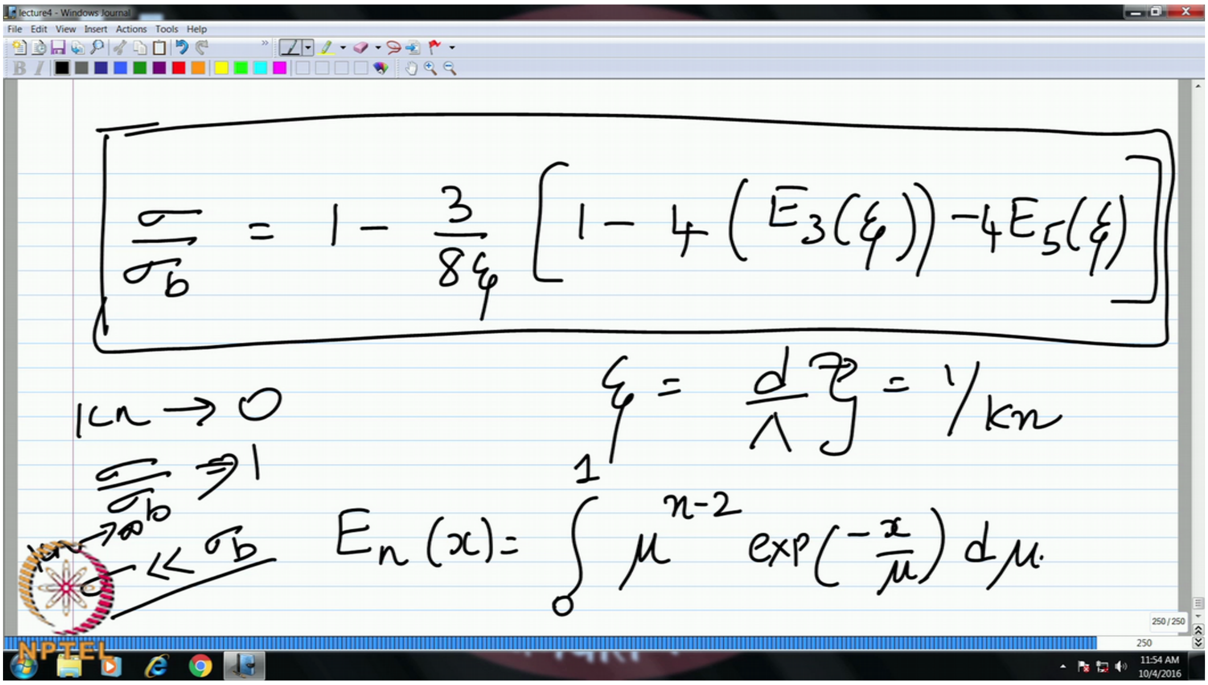

So, that will come out to be 1 minus 3 by 8. So, I am just using some notation I will expand what it is 1 minus 4 times e 3 of zeta. So, you can use some notation minus e 4 zeta.

and what is zeta this is nothing, but d by mean free path or this is equal to 1 over Knudsen Numbers and my e subscript n of x indicates integral 0 to 1 mu power n minus 0 exponential minus x by mu d mu. So, all I am doing is writing this product of v tau into mean free path and then, I evaluate these integrals and I will leave I will end up with 0 integral terms 1 which is e 3, e 3 is nothing but mu times exponential minus x by mu d mu the other is e 5. Where I have mu square mu power cube mu cube exponential minus x by mu d mu.

So, I have to separately evaluate this e 3 and e 5 integrals. So, and then I get this resulting expression for ratio of sigma by sigma b. Therefore, So, this gives you the expression for the size effect in electrical conductivity for the nanosacle transport. If your Knudsen Numbers is very small, what happens to zeta term very large and therefore, this entire term vanishes. So, for the case of Knudsen Numbers going to 0, what have happens to sigma by sigma b goes to 1. So, it requires your bulk electrical conductivity now when your Knudsen Numbers becomes, very large what happens your sigma will be not smaller than your sigma b. So, this is called the size effect I hope all of you are able to follow this. So, we have derived from the first principle using the Boltzmann

Transport Equation although it is a very t d s process we saw that, but this is a simplest possible analytical solution for describing the size effects, from which clearly it says that if your Knudsen Numbers the vanishing limit of Knudsen Numbers your electrical conductivity becomes your bulk value for larger values of Knudsen Numbers your electrical conductivity smaller than, you bulk value; that means, if you plot if you make a plot of this ratio sigma by sigma b as a function of Knudsen Numbers.

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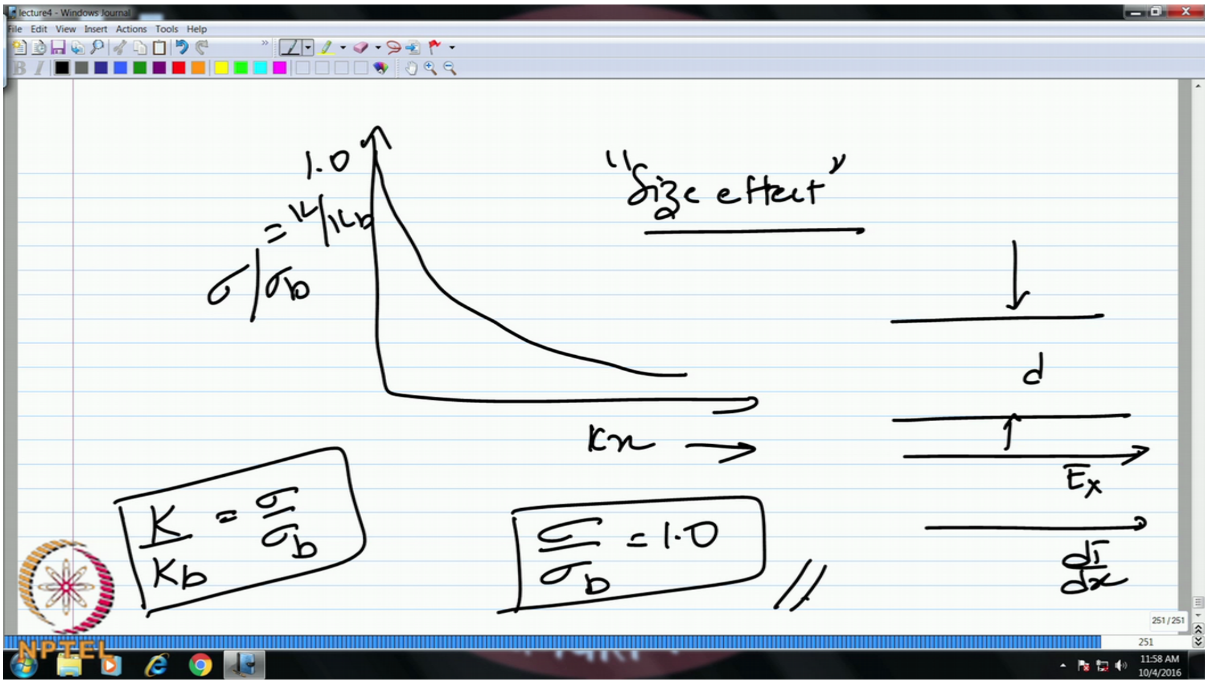

So, it is starts from one and then goes like this right. So, this is called the size effect. So, a nanoscale transport where is a reduction in the electrical conductivity even for the case where your transport of electrons is along the thin film and you have a confinement perpendicular to the transport even in this case there is a size effect seen because, of the scattering from the boundaries. So, this scattering is going to reduced the momentum of the electrons and therefore, it is going to also reduce the amount of electron conduction.

Now, what happens if instead, similarly if you calculate also the phonon if, you replace now with these electrons with phonons and you have a temperature gradient in the x direction. So, you have instead of electric field we can have temperature gradient and we have heat conduction parallel to the thin film and we have confinement perpendicular to that. So, in that case you can calculate the ratio of k by k b which gives you the size effect for thermal conductivity it turns out to be it will be exactly equal to similar expression as sigma by sigma b, you can do this as an excise and see that in this case you do not have any electric field you have only temperature gradient follow the same steps instead of electron charge flux you replace this, with heat flux and you will end up with expression which is identical to sigma by sigma b. So, you have a similar size effect for also the thermal conductivity.

Now the interesting question is what happens if you use specular boundary condition instead of diffuse in turns out? If you use specular boundary condition that the ratio of sigma by sigma b will always be equal to one for transport parallel to the thin film or in other words specular boundary condition does not affect the momentum of the electrons or phonons. Therefore, even if you have a confinement and if you apply a specular boundary condition this is not going to destroy the or reduce the conductivities.

Tomorrow I will show you simply how this happens for specular boundary condition. So, with that you will be able to understand that this size effect becomes very important in the transport parallel to the plane only if you have a diffuse boundary condition whereas, if apply specualr boundary condition there is no change in the conductivity parallel to the confinement. So, we are talking about now all these conductivities which are in the direction of transport which are perpendicular to the confinement.

Now the other case is where we have size effects in the direction of confinement there irrespective of whether you use diffuse or specular you will always have size effects because the direction of the gradient and in the direction of change in the non equilibrium are in the same direction irrespective of whether you diffuse or specualr boundary condition there is going to be therefore, an effect of this confinement.

So, this is a most important property of nanoscale energy transport. So, if you are working at small Knudsen Numbers you will not be one seeing this effect, but at large Knudsen Numbers s this becomes very prominent.