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Lecture-27 Nanoscale Energy Transport in a Thin Film-Part I

Good morning everybody and today this will be the last few lectures on nano scale energy transport. Since we do not have too many analytical solutions at large (Refer Time: 00:42) numbers, will take up 1 or 2, very simple cases for which we can find the analytical solutions and then I will give computer assignment. That will be what you are working on even in 1 dimension you know. 1 dimensional transport of phonons for example, using Boltzmann transport equation and you can for which we have the analytical solution and you can compare it with your numerical solution and understand how to solve this kind of type of equations. The Boltzmann transport equation is an actually integral differential equation. This is not something that you come across in a normal partial differential equation course and also the fact that it is dependent on so many dimensions. Even in 1 dimension, you are not solving only 1 dimensions space. You are also solving the directional space.

Therefore, it becomes 2 dimensional and therefore, even in 1 physical dimension, you have to solve with 2 dimensions therefore, that itself is computational intensive and when you go to 2 D and 3 D, it becomes function of you know 7 co ordinates and so on. It is a rigorous solution but at 1 dimensional level, you can try to find numerical solutions and also we have analytical solutions at study state. You can try to compare your results. That is the good way to probably you know conclude the you know discussion on nano scale energy transport. There are also more advanced concepts pertaining to you know composites you know nano composites and so on, but we will not cover in this particular course and there are also researches, research going on in for example, calculating the thermal conductivity of nano structures.

As I said in the case of bulk materials, the thermo physical properties are invariant and what is peculiar about the nano structure is the size dependents of this properties and therefore, we call this as the size effects.

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This is a very typical word used at it nano scales to denote the dependence of thermal conductivity and for example, electrical conductivity, if you take you know electron charge transport. All this function of thickness of the material that you are considering and you can also show that to the limiting case, where you have a very small Knudsen numbers. This approaches your bulk values. When we are talking about nano scale heat transport or in any energy transport, you generally refer to what is called the size effects and let us study 1 such size effects. We can first start with for example, with the electron transport and; that means, the flux of the charge, flux of current. This is your current flux which gives you the electrical conductivity and therefore, we can first understand the size effect with respect to electrical conductivity and we will see analogs to that how the thermal conductivity also exhibits size effects. To do this, now we are therefore, talking about real nano scale transport.

I mean although we were discussing many things about nano scale right before in the beginning, the real nano scale transport starts here. All this till now is to put the perspective on different kinds of subjects such as statistical thermo dynamics, quantum mechanics, all this are the fundamental building blocks and we finally, showed that for transport process the Boltzmann transport equation is the fundamental equation and from which we can drive all the classical constitute of relations. These were not really nano scale in that sense. The real nano scale transport will be dealing with now in the next 1 2 or 3 classes. To do this, again let us go back to the way we are deriving our continuum equation.

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In that case, we assume a quarter pation functions, distribution function from the, which is the difference between the non equilibrium and the equilibrium distributions and if you substituted this in terms of G and F equilibrium in the Boltzmann transport equation. You were having terms which involved G and F equilibrium. You had D G by D T D F equilibrium by D T plus you had also the gradient with respect to position for both G and F equilibrium as well as you had the variant with respect to the momentum space for both of them and then finally, on this side you had G by tau, scattering tau. The scattering term is approximated by means of the B G K relaxation time of approximation.

This is your Boltzmann transport equation, I think all of you should know this by heart and therefore, you should be able to write this at any point of time you know. We also made several assumptions in deriving the continuum equations as I said that if you look at the order of say D G by D T and D F equilibrium by D T. In comparison to the scattering term on the right hand side, these are much smaller correct or in other words we said the physical time scales or much greater than your relaxation time scales. Therefore, we can also call this in the in a sense that we are looking at more like a study state process we are not bother about variation of this distribution of time therefore, we neglected the time variation and we also invoked the assumption that your G should be smaller compare to F equilibrium and also the respective gradients of G should be smaller than the counter parts for F equilibrium. Similarly with the gradient in the momentum space invoking all this.

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Therefore we wrote your F in terms of F equilibrium minus tau into V dot l R F equilibrium plus F by M. This was the underlining transformation of B T. The actual B T is quite complex from there, we put all this assumptions and then we converted this to this form, which we use to derive all the continuum equations.

But; however, now when we are dealing with nano scale transport, we are talking about in the present case, we want to study transport in nano structures. In that case we cannot make all this assumptions. Of course, we have to make certain assumptions to solve them for the nano scale problem as well, but we cannot make this kind of assumptions what are the assumptions suitable for this problem. One is we can still make the assumption with respect to the time scales because we can say that although your Knudsen numbers are high, we are looking at problems where the physical times are greater than the relaxation time. That means, we are not looking femtosecond, picoseconds, laser radiation kind of process here. We are looking at clearly size effects, size effects coming from reducing the size of the structure not due to disparity in the time scales. Therefore, still we can make the first assumption that D G by D T D F equilibrium by D T. These are much smaller than the collision term on the right hand side because this is still valid.

This is 1 one important assumption. What is the other assumption that we can make? If

you look at the term F by M del V G, this is the variation are this is the gradient of the pet robe function in the momentum space, we can say this is also small compared to the corresponding change in respect to F equilibrium. If you make these 2 assumptions, the D T can be rewritten in Cartesian coordinates, 2 dimensional Cartesian coordinates. We neglect the unstudied terms. We have only the advection terms both in the physical space and momentum space. The first term we have V dot del R F knot, if you expand this we have V X D F equilibrium D X plus V Y D F equilibrium by D Y and similarly for G we have V X D G by D X plus V Y D G by D Y and the other term, which is important is D F equilibrium by D V X plus F Y by M D F equilibrium by D V Y this is equal to minus G by tau.

In other words by invoking the second assumption here, we also say that whatever deviation function or perturbation function could be quite large in the physical space because this is a nano scale phenomena you know. When you are talking about very high Knudsen numbers, you are non equilibrium function is suppose to deviate quite a bit from your equilibrium function. But this effect comes only with respect to the physical coordinate and not in the momentum space. This is therefore, a very important assumption. With that assumption, we reduce the dimensions, number of dimensions for G. G therefore, is only a function of X and Y where as F equilibrium is a function of X Y V X and V Y. So, this is your starting point and let us now considers 2 kinds of transport.

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One is we can talk about transport which is parallel to thin films. Thin films are the nano scale, nano structures. You can talk about a nano structure like this. You have a separation. This is your film; the film is thick with units of D. This is your thickness of the film here. It could be the order of few nano meters, for example, and your coordinate system is attached to the bottom plane and you have a momentum space which is $V \times V$ y and this is your V vector which makes an angle, let us say theta with a vertical. I mean this is your convenience if you choose theta here; you can choose the projection of this on to this plane and make an angle phi with the horizontal. It is up to you in the other case we choose theta as the angle with horizontal and then the projection on to the vertical plane making an angle phi with the vertical line. Now we are just picking for this convenience you can also do the other way.

Now we are talking about a temperature gradient which is not in the vertical direction, but in the horizontal direction. In this case you have a temperature gradient or you can have gradient of the thermo energy level and you can have corresponding electric field. In this case therefore, you maintain a temperature gradient or a gradient in Fermi level such that electrons move along the X direction. This is a case where your transport is happening parallel to the films. Your film is actually like this confining the film by dimension D, but the transport is happening along the film. The other case, where you study your heat transport and all that is 1 plate the bottom side is at 1 temperature top side is another temperature.

In that case, transport is happening perpendicular to the film but this 1 of the simplest case you can start with transport parallel to the thin films in that case. Now, let us draw the momentum space separately. You have $V \times V \times V \times Z$. This is your momentum vector and this is your polar angle theta. Now polar angle we are defining as angle with respect to the vertical coordinate V y and the projection of this on to the bottom plane the V \bar{x} that plane. That will make an angle phi, the azimuthally angle with respect to the X coordinate, V x coordinate. And therefore, now let us look at the terms D F equilibrium by D Y. Now with respect to F equilibrium, now F equilibrium is a function of your x y V x V y according to the equation that we have written here yeah. Now, in the case where you have transport parallel to the thin film, what will be the most important function, F equilibrium variation in the X direction, or Y direction; in the X direction because we have transport in that direction.

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Therefore, now when you talk about D F by D F equilibrium by D Y, we can actually assume this is smaller than the corresponding deviation function gradient in the same direction. You have very strong gradients F equilibrium varying with X because of either the temperature dependence or because of Fermi level dependence on X.

However, if you look at the variation of G, in this case, G will be very strong function of Y. Therefore, in comparison with D G by D Y we can neglect D F equilibrium by D Y on the other hand if you are looking at D F equilibrium by D X. So, this will be quite strong compared to D G by D X. Therefore, now this are again we are made already couple of assumptions here 1 2 and brought to this form, now for the case of transport parallel to the films we make assumption number 3 and 4. Depending on the direction of the transport, you can say what will be the order of magnitude of the derivative F equilibrium in the X direction it will be very important significant, where as in the Y direction it will be non-significant. Therefore, when you write down let us say this is your equation number 1 and reduced for the case of transport parallel to the film, can all of you write that down?

We have D F equilibrium by D X very dominant, second term will be less significant, the third term also will be less significant and then we have the fifth and sixth term out of these 2 again, when you talk about D F equilibrium by D V X D F equilibrium by D V Y which will be more significant. We have transport along the X. Therefore, the external force which will be acting the electrical field or whatever it will be acting in that direction. Once again we can ignore D F equilibrium by D Y comparison to D V Y comparison to D F equilibrium by D V X.

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With all of this assumption for this case, the D T will reduce to therefore; it depends on scenario, if you are now looking at the other case transport perpendicular to the film.

If you maintain therefore, a temperature gradient or maintain an electric field in this vertical direction in that case, how will you reduce this equation? When you talk about D F equilibrium, in which direction will be the gradient? In Y direction, This will be the greater corresponding to D G by D X D Y sorry and similarly if you are talking about D F equilibrium by D X this will be much smaller in comparison to D G by D X and similarly, D F equilibrium by D V Y will be great larger compared to corresponding derivative here.

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Therefore, for this case, you get V Y D F equilibrium by D Y plus I think let me just make sure I think the right terms here. This should be V X. I, this should be X D G by D X plus I have F Y by M D F equilibrium by D V Y should be equal to minus G by tau. I think this should be fine right now.

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What we will do first? Let us take the first case the phonon transport or electron transport parallel to the thin films. We will take the case 1, transport parallel to thin films and can you try to solve I mean what I can give you as a hint now, take the equation number let us call this number 2. We have D F equilibrium by D X; you have D G by D Y D F equilibrium by D V X. Now, let us group these terms. 1 side, left side we will group the terms with respect to G on the right hand side we will group the terms with respect to F equilibrium. Can all of you do that? You group that and write the right hand side terms which are functions of X for example, $D F$ equilibrium by $D X$ we have $D F$ equilibrium by D V X. So, you can write this as some function of X and then try to get the solution for that particular differential equation just attempt it.

Write 1 side of function of Y the other side function of X and whatever we have $D \nabla F$ equilibrium by D V X D F equilibrium by D X. These are just some function of X. You group all of them as 1 single function of X and then you try to solve the O D with respect to Y. I hope you could get to this point now right. I am writing on 1 side function of Y, G is a function of Y and the other side F equilibrium as a function of X. All of this on the right hand side together, we have 1 functions of X, the reason why we are doing this. In fact, is that now when you take thin films and parallel to that it is not very obvious whether there will be size effects in this case because you have a confinement in the direction which is perpendicular to the transport? You might wonder if I have a transport in this way, how this confinement is going to bring size effect.

But what is happening in nano scale is that we are talking about now scattering of phonons or electrons. Not only electron, electron scattering, but electron boundary scattering is happening. This is going to bring about distortion of the equilibrium non equilibrium function quite substantial, even when you have transport along the plane along the film the distortion can happen in the perpendicular direction because of this scattering mechanism. That is why we say that D G by D Y is still strong here.

Your D F equilibrium does not change with respect to Y; however, your D G by D Y we cannot say that because D G by D Y is the reason why we are getting a size effect for this case now there, where as a if you look at the transport perpendicular. So, there is a small correction that you have to make. So, the transport perpendicular it is very clear if you have a temperature gradient in this direction and you have a confinement in that direction. Your F equilibrium is going to vary in that direction and so is your perturbation function. Perturbation function is also very strongly dependent in that direction not D X. Please correct that. Therefore, we do not have D G by D X term here. It will be D G V Y D G by D Y. What should be ideal case the way I have written here? This should be large and you can say that, this is small and you have D G by D X approximately 0 because in this case the distortion or perturbation cannot happen along X for a case you have transport perpendicular to the plane. I hope you are able to understand the point. So, when we now do the solution you will be able to get this fact, but what you have to understand right now is when we start the problem, where are the nano scale effects coming from?

When you talk about transport parallel to the thin film, in this case the distortion function still has to varying along Y. That is what is bringing the size effect. When you are talking about transport perpendicular to the film, already the confinement is the Y direction, the transport is also in the Y direction, the distortion function will be vary along the Y Y direction. There is no variation of distortion function along X. In that case, your D G by D X will be 0, you understand, but still when you are talking about transport the F equilibrium will depend on the direction of the transport, but not the perturbation function, in the case of transport perpendicular to the film. You please correct it; it should be V Y D F equilibrium by D Y plus V Y D G by D Y.

Both the distortion function and F equilibrium will vary along Y, where as in the transport parallel to the films you are F equilibrium varying along X distortion function varying along Y, but without that variation of distortion function along Y, there will be no size effects. That is 1 which is causing size effects even when you have transport parallel to the films and we will see how it is happening that is because of boundary scattering. So, now, when you therefore, write this equation for thin films parallel transport parallel to the films, we are grouping this all the Y terms on the left hand side all the X terms because what we are more interested is to find the solution of G as a function of Y and this is what contains the size effects information in it.

Therefore, we for the sake of solution we will just combine the terms with respect to X as 1 function of X, for solution with respect to Y, this is not required that can be just added as it is at the end. With we are more interested in seeking solution with respect to Y and especially for G as a function of Y and therefore, when you solve that. Can you solve this particular O D E now? We have this is equal to minus S knot of X. This is your O D, where you have non homogenous term. There will be a complimentary function there will be a particular integral, the complimentary function will be the solution to the homogenous differential equation. What will be that function?

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That will be tau V cos theta into D G by D Y plus G equal to 0. This will be the solution to the homogenous o D. The solution comes out to be; can all of you please quickly work out and tell me? G is a function of Y. We can say C exponential minus Y by tau V cos theta.

This is where the actual size effect is coming from. You are confining your Y direction. You are confining this with few nanometers. This is where the distortion of G is happening along Y and this is going to bring in the size effect for electrical conductivity or thermal conductivity. Therefore, now if you add also the full solution will be complimentary function plus particular integral now is a function of X, does not depend upon Y. That can be just simply added on to this. Therefore, you will get the final solution of G G of Y plus S knot will be equal to C exponential minus Y by tau V cos theta. You keep this solution right now and mean while we will find out the expansion for this S knot. Now we know already that S knot term is basically this. You have D F equilibrium by $D V X$; you have $D F$ equilibrium by $D X$.

Just like we did it yesterday's class, we can expand now D F equilibrium by D X as D F equilibrium by D E F or D T in this case. Let us say you considering only transport of electron flux, current flux. Therefore, this is the dependency of Fermi level on positions. We can write as D F equilibrium by D E F into D E F by D X. Similarly if you are talking about D F equilibrium by D V X, it is a function through E D F equilibrium by D

E into D E by D V X because of the dispersion curves. Dispersion curves give you relation between energy and the momentum, the same way that we did yesterday.

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If you do that, the expression for S knot of X will be minus and you substitute for the force, Lorentz force charge time's electric field. It comes out to be minus E times tau V X D F equilibrium by D E into E X plus 1 by E D E F by D X. Please check this with yesterday's expansion. We also use the fact that your D F equilibrium by D E F is equal to minus D F equilibrium by D E. I asked you to check that. Did you check that? Different take the derivative of Fermi direct distribution function with respect to D F with respect to U and check. There will be same in magnitude opposite minus the, did anybody check that? So, you are convinced. All you could reach to this point. You have a solution with respect that G of Y plus S knot. S knot is a function of S X and solution for S knot is already known. It is a function of F equilibrium.

Now here is where we understand try to understand what is happening to the scattering of electrons. Now, when you talk about whether it is transport parallel or perpendicular, inevitably you should talk about scattering of electrons at the boundaries because this is where the confinement effect makes the difference. If there was no confinement, this scattering from the boundaries will be very negligible. Electron - electron scattering will be more predominant over electron boundaries scattering, but when you are now talking about a confinement that you bring in, does not matter you whether you have transport this way or this way, now you are going to have electron which come because as you see from the solution to the B T electrons can travel in spherical coordinate system. It did not travel only vertically up or horizontal.

It can travel in sphere encompassing in all directions of a sphere. There can come in any direction. Electron which is coming like this will hit the boundary and it will change the direction, similarly electrons which come to the bottom boundary will hit and change direction. Therefore, this process of electron boundary scattering is the 1 which is causing gradient of the perturbation function along Y. Even for transport parallel to the plane, if you for example, therefore, look at the scattering mechanism from the bottom boundary, we have assumed the coordinate starting from the bottom Y and we have the scattering electron from the top surface.

When with respect to the coordinate system that we have taken for we have V X V Y. V vector. We have taken theta with respect to the vertical. Therefore, what angles of theta does this scattering from the bottom correspond to theta going from. You can, when you are talking about variation of theta. Theta 0 starts from here and then you are talking about 0 to pi by 2 and then pi by 2 to phi. When you are talking about therefore, scattering upwards direction, what is the variation of theta? 0 to pi by 2; and what about the downward scattering? Pi by 2 to. Is that clear? This corresponds to the scattering in all these direction. This is your upward direction where theta can vary from 0 to pi by 2 and now if you talk about scattering in this direction downward direction your theta can vary from pi by 2 to pi and the other half is coming because of rotating phi.

Now you are talking about a sphere. Your theta varying from 0 to pi and phi varying from 0 to 2 pi. You first swipe a semi circle and then rotate it about the vertical axis or correct. That will bring a full sphere. Therefore, we have these direction cosines here. In this case direction cosines will be positive. Cos theta and in this case it will be negative. We will call this part, which is scattered from you know which is moving towards the positive in the positive direction cosine space as G plus and the solution which is moving in the negative direction cosine space G minus. I hope all of you are following this. We have this G as a function of not only Y. In fact, it is a function of cos theta as well.

And therefore, we have scattering of G going in all direction, even for 1 dimensional problem. We are segregating, we are breaking this into the ones which are going up scattering and going up the other which are scattering and going down we call this as G plus and G minus.

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The same solution, therefore can be written as, you can say that G plus will depend on Y and the positive direction cosine space can be simply S knot exponential. I have to do 1 more step here. The other thing is we have to apply from the boundary conditions in order to calculate the constants. Now, will have 2 constants for this case, 1 for G plus there will be a constant the other G minus will have another constant understand. Therefore, we have 2 constants we have to find this by corresponding boundary conditions. We have to understand, what is the characteristic of the scattering at the boundary? What type of scattering it is? There are 2 extreme possibilities, 1 is called diffuse scattering, the scenario I have depicted here.

An electron can come in direction, downward direction like this and the surface can be so rough, that it scatters in all the directions from the boundary. This is called diffuse scattering. In the diffuse scattering you have a uniformity of the emerging distribution over the entire directional space. All of these are uniform, equal, where as the other extreme is called secular scattering you have a perfect mirror image, you have like a polished mirror. It comes in a particular direction. It reflects like a mirror, mirror image you know direction which is making theta to the vertical. We will look at this 2 boundary conditions in detail in the next class, based on that we will calculate this constants, find

the solution and we have still not got the final solution, solution is only for G. Now we have to use this to calculate the current flux, the way we did in yesterday's class. Only difference is yesterday we were doing it of continuum case and now we are doing for nano scale case.

So, we will stop here.