Micro and Nanoscale Energy Transport
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Lecture - 22
Non equilibrium energy Transport at Nanoscales: Boltzmann Transport equation

Today we will look at the actual transport phenomena. So far we are focused on basically the equilibrium process that is looked at thermo dynamics from the statistical point of view, and also little bit about the transport process from the kinetic theory point of view, but in order to move towards more regress transport process.

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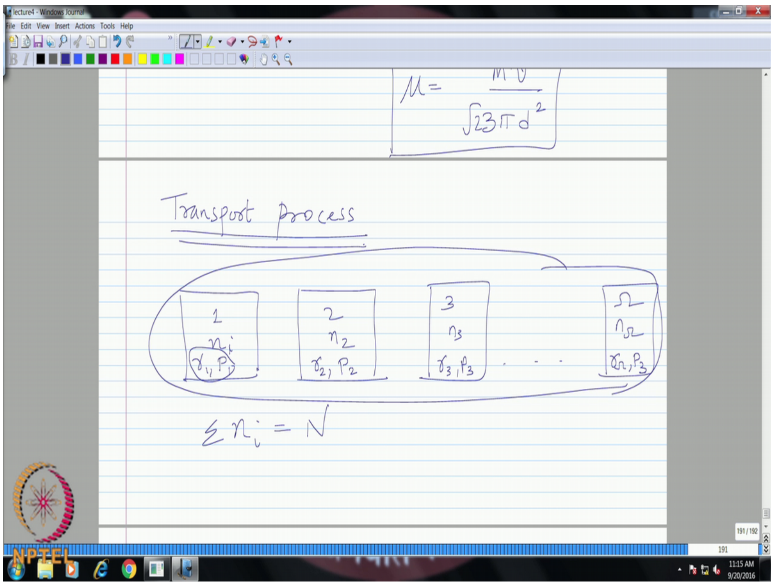

So, if you want to understand how the transport process has to be studied. So, first thing you have to know about again this is the distribution function. So, in the case of the equilibrium thermodynamics, so, we looked at different quantum state and then the ensemble of that, and we said there is the definite number distribution for each of this quantum state if you have for n number of the particles. So, particular quantum state this could be quantum state 1, 2, 3 and so, on.

So, we have so many number of quantum states and then you have a particular number distribution n subscript i for each quantum state. So, we have n 1, n 2, n 3 and. So, let us say this is last quantum state we have n subscript omega. So, therefore, if you take summation of n i this will be equal to total number of particles n which as distribute across all these quantum states.

So, this was common in both the equilibrium whatever we have studied and also what we are going to study in case of transport process; however, the differences that in the case of equilibrium, each of this quantum state of particular energy value associated with these right. So, we talked about therefore, e i e 1, e 2, e 3, e 4 up to e omega, but this is not sufficient to describe transport process see apart from your values of energy and corresponding equilibrium distribution function that the part given energy carrier can take, we also have to understand for a transport process there has to be advect to.

Therefore, there are certain values of equilibrium distribution function which holds for systems equilibrium are when there is no transport, but if there is the transport process. So, how do we describe the distribution function now? So, of each of the quantum state now instead of describing this with energy levels, we will have to move and use the position rector r the particular quantum state can have a particular value of position rector that is in a point in space. So, it can be actually located at some position and it can have particular value of momentum.

So, this is what in going to distinguish the actual transport from the equilibrium case. So, each of this quantum state is now going to be represented with the value of the position vector and the corresponding value of momentum vector. So, this is a more complex scenario that we are considering. Therefore, if you are plotting a diagram where we plot the momentum vector in a vertical coordinate and then have the position vector, on the horizontal coordinate now each of the quantum state is represented by particular dot here.

For example, quantum state 1 could be this quantum state 2 could be this, quantum state 3. Like that I can put all the points each point representing quantum state and plot this on to this map and therefore, a collection of all these quantum state will one and some. So, whatever I have represented here.

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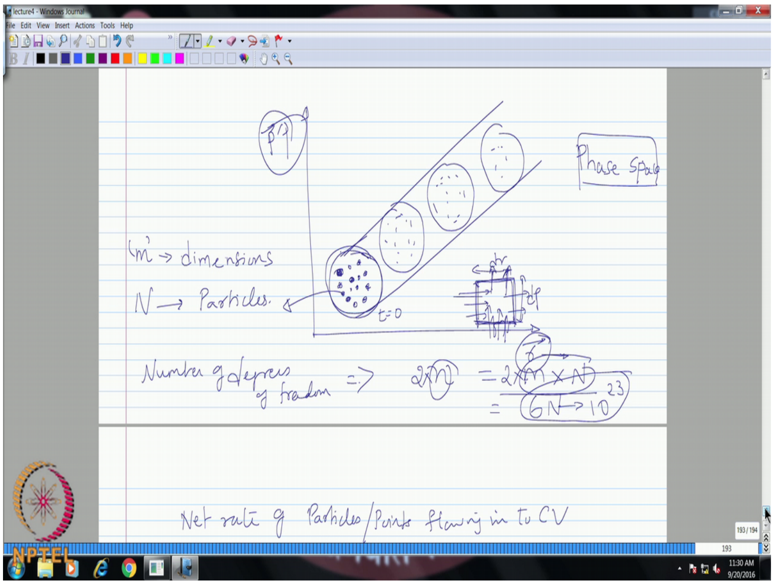

So, 1 to omega number of quantum states each representing value of position and momentum. So, if have plot them on to this map of p versus r. So, have discrete points and, if I describe the ensemble of all this together. So, that will be the contained with this particular circle.

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It should be can be started it can be, but not. So, widely because what we are saying this each quantum states is more or less moving with the you know similar velocity, and position it is not completely off now how do we talk about transport here therefore, we want to look at an ensemble of collection these particles occupant different quantum states finally, have to advect, when they advect; that means, this ensemble has to keep moving in time. Therefore, if you start from time t equal to 0 we will have an ensemble which is representing like this and now due do advection after certain time then this ensemble would have travelled to this point in the this position in the p r diagram.

Similarly, after certain time if the collection of these particles would have had a different value of momentum and position and. So, on this is now going to therefore, travel like these with a definite velocity if there had been no velocity this would have been just here. So, this is basically you can probably think of some similar to the equilibrium distribution function, and now what is distinguishing the transport process is that you have a advection happening and therefore, there is a change in the momentum and position vector with respect to time which as to be now tracked, and accounted for and again the collection of these particles keep changing. So, these ensembles itself keep changing it is collective momentum and position.

Therefore, we have to study not only the average energy that is possessed by this ensemble of particles, but also the relative motion and momentum. So, this have to be studied with respect to time and this will give you information about the transport process. So, this on a very fundamental level and this kind of diagram, where you plot your momentum vectors position vectors is called a face diagram, or phase space you should understand this is a multi dimensional space which we simply plotted as p versus r because r is a vector. So, this itself is a three dimensional space and momentum will also vector which again a three dimensional space right.

This we have just squeezed into some kind of a two dimensional map, and we have trying to look at the transport. So, this kind of diagram was called a phase diagram. So, therefore, if you looking at each particle. So, how many let us say if you are talking about this is your let us say. So, this is the degrees of or dimensions we can distinguish this your degrees of motion we will call this m dimensions these are your dimensions that we are going to look at could be one dimension, or two, or three and if we have totally n numbers of particles the ensemble what is the total degrees of number of degrees of freedom.

So, let us say this is n this is the total number of degrees of freedom small n. If you have m dimensions basically m times n when you are talking about for example, just only the position, it can move in a long time in translation x y z for example. And therefore, each particles can have three degrees of freedoms therefore, n numbers of particles system of n numbers of particles when m into n degrees of freedom. Now if also looked up momentum, momentum also are there in three directions x y z if you also include that the total number of the degrees of freedom will be 2 times.

So, if you are including both the advection position also as well as the momentum into the degrees of freedom the total number of degrees of freedom, that you have 2 times m times n if you are talking about three dimensional space therefore, this is 6 times n, n could be a large number of particles. So, if you are talking about (Refer Time: 11:31) number 10 power 23 for example, you are talking about therefore, tracking an ensemble of 10 power 23 order of magnitude particles within time.

So, this is not a very simple task. So, we will come to that. So, now, what we will do is write down for example, the equation of conservation of this particular transport process. So, if you take a control volume in the d r space. So, this dimension could be d r in this could be d p, and what we are going to do is apply the flux conservation principle, here that is the net rate of particles or points whatever you want to say because each dot is now 1 quantum state represented by n i number of particles .

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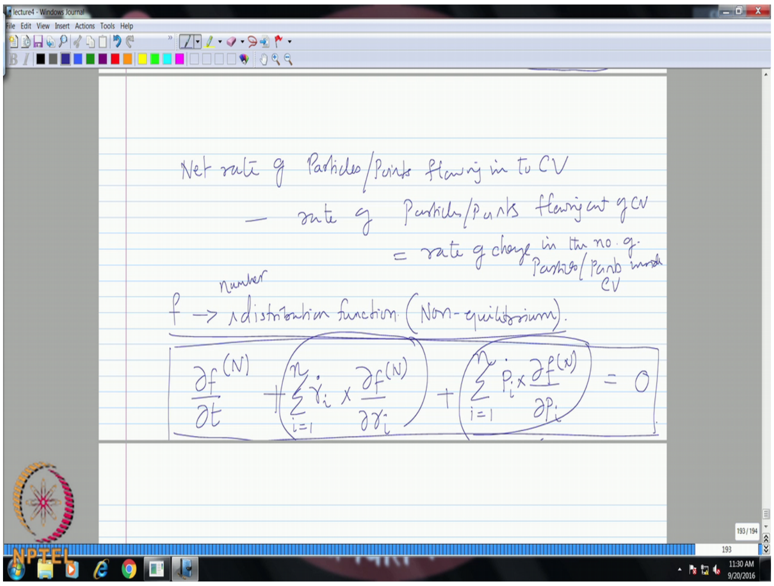

If you are therefore looking at the control volume boundaries you are looking at all these particles which are a collection of all these points which are collection of particles basically entering and leaving the boundaries of the control wall. Therefore, if you want to write down the conservation equation we say the net rate of particles are points flowing, into control volume minus the rate of particles or points flowing out of control volume should be equal to rate of change in the number of particles points inside control wall. This is like your mass conservation, just like your mass has to conserve in the case of study state whatever flowing in should be equal to flowing out, similarly now you have a number distribution, now if you take particular control volume and apply the conservation of this number distribution. So, you have this number of particles which are our points which are entering this should be equal to something going out and something which is changing within the control wall

So, if you have expand this to mathematical form, we can write this as if you represent m f as the number distribution function, which you already are aware right this is your particle number distribution function only difference is that in the transport process this is a non equilibrium distribution function. Whereas, in the case of statistical thermodynamics this was an equilibrium distribution function, since now you are studying transport phenomena this has to be a non equilibrium, then only you have a transfer process. So, f is now becomes non equilibrium distribution and therefore, it will become a function of r and p right position and momentum.

Therefore, if you write this mathematically the conservation equation will be d f by d t; this is your rate of change of the particle distribution within the control volume. So, this you are writing for a system with n number of particles. Therefore, you have to use the superscript n, to do not how many number of particle system you are dealing with plus, now you talk about the advection process right. So, if you are doing a lagrangian tracking that is you are looking at this particular ensemble and then tracking its motion. So, it is primarily only with time whereas, if you have a fixed control volume like this in space. So, this becomes an oilarian motion.

So, relative to this fixed volume you are tracking about the motion of these particles. So, therefore, you have a change with respect to position as well as momentum right. So, therefore, first derivative will be the rate of change with respect to the position which will be d f, by d r. And now r is basically a vector. So, in the tonsorial representation you can use r subscript i, you are tracking in each direction and again this f is the collection of n number of particles and the velocity here, will be what does to advect in the position with a definite velocity.

So, that is basically d r by d t you can use our subscript i dot. So, the product of this and now this has to be summed over all the 1 2 n, because now you have n degrees of freedom. So, you are talking about a n particle distribution function therefore, the number of degrees of freedom in all the three directions will be m cross n if you are talking about m dimension, m dimensions, n particles. So therefore, this has to be summed over all of them you cannot individually track each particle, you know each coordinate space and write the conservation, it has to be completely for the entire because is r 1 2 3 represents each direction now it is clubbed together a single r, that is what we have drawn as p versus r diagram here and similarly p. And now each particle will have definite location coordinate.

So, we cannot look at each particle again. So, we have to look at ensemble of particles. So, for this ensemble with n number of particles basically it has to be having n degrees of freedom. So, it has to be summed over all this and this collectively should represent the advection with respect to space the other is the advection with respect to the momentum. So, we are talking about therefore, change in also the momentum as it is getting adverted. Therefore, we will have a similar derivative with respect to the momentum space p, and again for the momentum space also we have n degrees of freedom totally and this is your derivative of p, so, again p subscript.

So, this is the second derivative which is coming from the advection in the along the momentum plane. So, all this should be equal to 0 rights. So, therefore, this is your conservation equation, if you represent a small rectangular control volume like this and use the oilarian frame of reference you can write down the change in the number distribution, what is happening in the position space in the momentum space and this is your conservation equation. So, now, how easy is it to basically solve this equation?

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Here, now here it is the number total number of degrees of freedom. So, we have m dimension for each particle and we have n number of particles. So, total number of degrees of freedom is small n which is m time's capital n.

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For each quantum state need not be there is a distribution function for an ensemble it is collection of all these quantum states you have n particles capital n number of particles. So, for that ensemble is what we are actually concerned about. So, this ensemble will have a distribution function f, which is basically changing in time with position and which moment.

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Correct, so, you know you are right. So, what we are saying is now for each particle. So, the way we are looking at this. So, you what you are saying is for each quantum state there is a particular r i or b i or for each particle you are saying.

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Correct.

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So, this is one microstate you can call this is again a small micro ensemble.

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The n must be constant for the macro ensemble. So, that is for this collection. So, now, what you are saying is now each microstate has n i particles. So, within that you have the particular distribution so; that means, one particle will have a particular position and momentum, another particle will have another one and this collection is basically your n i which is a micro one microstate, with a particular representative momentum and position . So, you can actually look at this break down into each value of momentum and position, we are representing this with one quantum state which is a microstate micro ensemble, and like this we have several micro ensembles put them together you have the macro ensemble.

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Distribution of energy is different, yes the actual if you look at the actual occupancy function. So, within this if you go within this you have a distribution function at different values of momentum and space position. So, each particle will take up a particular value of momentum and position and that is given by this n i.

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But what we are doing now, statistically we are not concerned about tracking each and every particles, motion and momentum you know. So, what we are doing is we are grouping this together you know into a microstate, into a microstate and we are representing that micro state with n particles having a representative momentum effective momentum and position. So, that is one dot like that we have. So, many micro states which are all given by each of these dots, now this together is an ensemble which is your macro state.

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Yes. So, we that are what I have written here, so, if you have three dimensional spaces you have 6 n.

Student: (Refer Time: 25:37).

No sorry for it, now this is for the math the complete ensemble of all the microstates that should took together should have the number of capital and number of degrees of freedom. So, we have n particles. So, capital and number of particles therefore, you have capital n times m degrees of freedom should be therefore, the entire ensemble, and this entire ensemble is now cutting across you know a particular oilarian in control volume, therefore it is going to get now transported.

So, it is less its position is changing due to a finite velocity its momentum is changing due to that particular value of force that is your rate of change of momentum. So, you are applying an external force which can actually result in change in the momentum plus, you can change the position due to its velocity due to the advection. So, we are tracking this particular ensemble and therefore, now we are not concerned about each and every quantum state, we have gone to now average or sum this over the entire ensemble of this microstate. So, that is why we are doing summation i equal to 1 2 the number of degrees of freedom totally

Actually, there is a much more detailed derivation of this which I have skipped through and made it much easier for you to understand, because most of you are already aware about how transport laws are derived. So, I am just giving an analogy with that to make you understand that finally, it is amounting to a conservation only thing now when you talk about conservation of say mass or momentum you are only looking at say two dimensional space, or three dimensional spaces. And therefore, you have only this particular term. Now what I am saying is we are representing this three dimensional space in one d axis, and another three dimensional space of momentum in another axis. So, therefore, we also have a second derivative coming from change in the momentum, momentum space. So, this has certain significance, so, I will explain that to you. So, this is basically your force the first term resulting in change of momentum, if there is no force this term becomes 0 and this becomes similar to your classical conservation equation, but what finally we are doing a telling is that if you want to solve this kind of an equation.

What you have to do is you have to track all the n numbers of particles and you have to also understand the degrees of freedom n degrees of freedom, you have to sum them over all the n degrees of freedom, which is computationally very, very rigorous. So, you have to keep track of all these micro states within the ensemble and also all the degrees of freedom and therefore, we should distinguish all of them and then finally, sum them up in order to satisfy this conservation equation. So, that is the way this equation can be solved and practically this is not possible.

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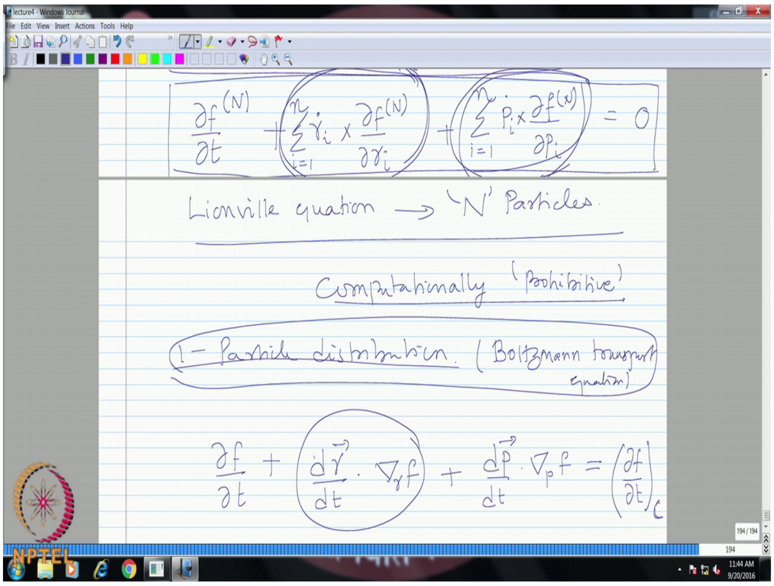

So, this kind of equation this is called as Lionville equation. So, the Lionville equation holds for a system with the n number of particles, and this is too cumbersome to track the distribution with n number of particles, the n particle system you have to track all the n particles you have to understand the distribution function for each microstate and then sum them over all the of freedom. So, this is going to be computationally prohibited. So, we can right away say this although this is your perfect equation this is computationally prohibitive to solve this therefore, the more practical approach is to reduce this to a 1 particle distribution function.

So, like we say you know, you in the represent if you take n particles out of that you pick only one particle and think this is the representative of n particles, like a sampling this is good enough to represent what the n particles distribution is and you assign this to 1 particle. So, now, this is going to be computationally easier, but you see the number of degrees of freedom have just reduced like anything, but what is computationally feasible to solve is to look at one particle distribution.

So, we have brought down all the degrees of freedom from n number of particles to 1 particle. So therefore, if you are looking at three dimensional spaces your number of degrees of freedom will be 3. So, from 10 powers 23 we have brought the number of degrees of freedom to 3, if you take 1 particle distribution function. So, for this the Lionville equation will turn out to be the Boltzmann transport equation.

However, has a downside; so I can simply replace this d f n by d t with d f by d t which is a one particle distribution function these all the summations will disappear now, essentially or the summation will have to happen in three dimension that is it, but what will happen since you have n particle system this conservation equation is perfectly satisfied, now if you remove that and you put 1 particle you do not have number consideration.

So therefore, in the process we have to now add another term which is your collision between the particles. So, when you simply reduce the degrees of freedom it is not simplifying maybe one part it is simplifying the advection part for example, but you introduce a newer term to satisfy the conservation equation then that is the coalition term. So, therefore, neglecting all the mathematical details I will directly give you how this 1 particle distribution will satisfy the conservation.

Now, the term here will be in three dimensional spaces. So, you have this will be r dot I, that will be u into similar to your valor. So, d r by d t in the x direction will be u velocity d f by d x. So, this can be simply written as what, like some velocity vector dot product with your gradient of the distribution function with position. So, this can be therefore, simply written as d r by d t. So, let me use the same notation as you know textbook. So, that. So, I just still use d r by d t and this is your vector dotted with your gradient in the r space of the distribution function.

So, this has now for 1 particle simplified to a simple term, which is your transport term. Now this is the other term which is with respect to your momentum space also can be written in a similar manner, dotted with del p f that means, you have 3 degrees of freedom essentially in each space, momentum space and position space. And you are finding the derivative in each direction making a dot product with your corresponding change of that quantity with time; however, this will not be equal to 0 to satisfy the number conservation there will be a term which I represent like this, but this is not a time rate of change, I use this entire bracket subscript c this means this is called the collision between particles.

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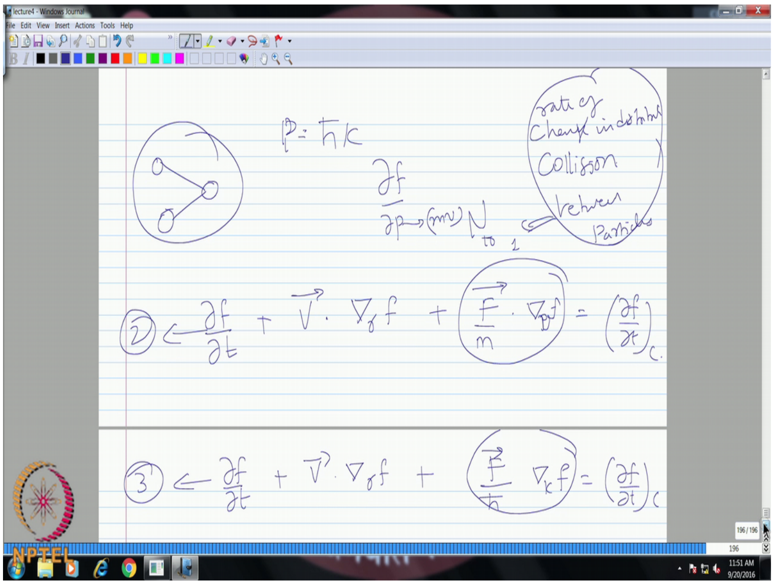

So, this is the change in the distribution function due to collision between particles a rate of change in the distribution. So, this has is coming, because of reduction from an n particle system to one particular system, but; however, we have greatly simplified the transport equation, which now can be solved or we can at least attempt to solve this right; however, due to the introduction of this collision term we have a lot of difficulties we will see that this collision term is not simple.

So now, we are talking about maybe collision between two particles and you have a third particle which is coming out and you can talk about collision between three particles, this is a more complex situation. So, it becomes a multi body problem right. So, it depends on how many number of particles you are actually looking at in a given time to solve this collision problem even a simple 3 particle problem that is two particles colliding and forming a third particle. So, two phonons colliding and you get a third phonon. So, two electrons colliding getting a third electron. So, even this is a very complex collision process you do not have a very simple expression to model this and we make a great deal of approximation to that.

Just give an example how the collision process looks like if you take for example, two particle scattering process like this. So, let us say before we go into that we can write two or three different versions of the Boltzmann transport equation, let me call this as equation number 1. So, this is your basic format we can also write this as you can see this is your velocity of the energy carrier with which it is advecting, right and this is your rate of change of momentum now what is rate of change of momentum force.

So, this is your force vector. So, the alternate ways of writing this is d f by d t plus you have velocity vector. So, just to distinguish the derivative with respect to the position space and the momentum space, I used dell subscript r and del subscript p. So, the other one is your force vector del subscript p. So, now, this is what del subscript p is actually d f by d p right. So, this I can write this in terms of velocities also I can replace p as m v. So therefore, I can replace this derivative with respect to velocity and I can bring the m out this is the mass of the particular energy carrier or particle.

This is an alternate way of representing the force term. So, this is say equation number 2, now there is also another way of representing this, we also know that if you look at wave particle duality. So, we from the quantum mechanics we have already derived the relations between the energy and the wave vector, and somehow we have used that also for particles. So, we had looked at electrons in a crystal we have looked at phonon. So, for all of this we have derived the dispersion curves which is essentially represented by relationship between energy and the wave vector.

Therefore, we can also keep moving from the momentum to the wave vector space because many cases we have the dispersion relation we can deal with the wave vector space. So, you can always deal interchangeably between the particle and wave aspects, and we can also write the force term with respect to the wave vector. So, how do we do that?

So, you have the force vector again you have d f by d p d p will be simply h cut k. So, we can write this as gradient with respect to wave vector space f equal to e f by. So, therefore, all these are the same Boltzmann equation only it depends on how you are writing the gradient of distribution function, when you have a force you can write this in terms of the actual momentum space, or you can write in terms of velocity space or in terms of wave at the space all these are equivalent, because momentum is related to wave vector and also to the velocity right.

Therefore, now in order to solve this equation you need to track the particle with respect to say three dimension, if you are doing this in three dimensions you have to calculate the derivative with respect to the position in three dimensions and with respect to the wave vector k x k y k z it. So, there are 3 dimensions of wave vector space. So, therefore, you have to account for 6 dimensions. So, 3 special coordinates, 3 momentum coordinates, and 1 time coordinate.

So, this becomes a 7 dimensional problem right. So, at least a 7 dimensional problem right now, so, therefore, still this is much better than looking at 10 power 23 dimensional problems, computationally this is possible to solve now the coming back to this collision term. So, as I was describing for a simple to particle collision like this. So, you have two particles.

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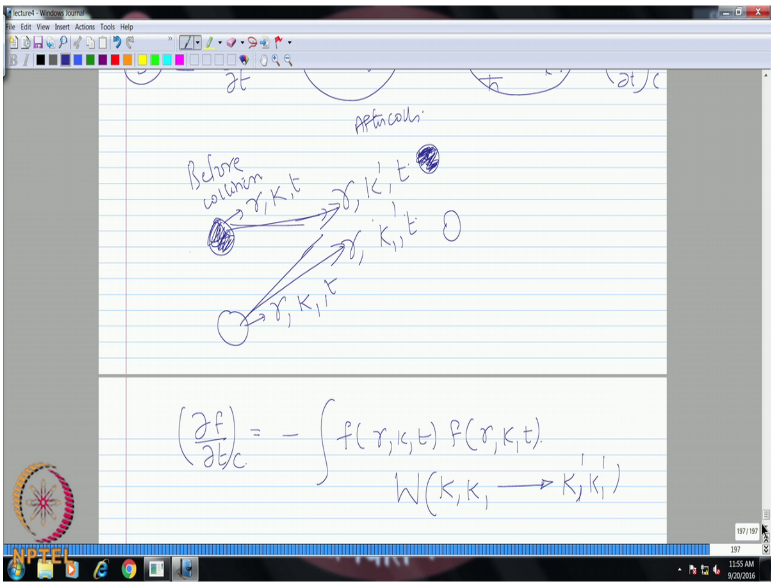

For example, you can say one particle has position r. So, and you have wave vector k for this, the other particle is also at the same position of these two are colliding with each other. So, position is the same, but different wave vector; that means, it can have different momentum different values of energy. So, at time t, so, after collision, so, this two will collide and a new particle is formed and this particle will have a value of position which is still r, but the value of k now can be denoted with k prime.

Therefore, you can write the d f by d t, if you do it in a slightly different way. So, I am assuming that these two are not simply colliding and forming a particle, but some kind of coalition which could be either elastic or inelastic, we are considering an inelastic system in which your momentum is going to change and energy is going to change after collusion. So, we can say before collision you have these two particles now after collision. So, this is going to change to r and will say k prime t and this momentum is going to change to k one prime t. So, this is particle let me shade this particle one, and this is also particle one after collision, this is your particle two before and after collision.

So, that is there is also scenario where these two particles can collide and effectively you represent this by a third particle with an effective value of momentum and position , but in this scenario we are just saying the same particle before and after collision will have a change in the wave vector from k to k prime, and the second particle will change the wave vector from k one two k one prime therefore, the collision term for this case is written as minus integral you have f of r k t this is for your particle one before collision times f of r k 1 t, this is the second particle before collision and you have a function. So, this function I will come to this, I will explain what it is we have k comma k 1 before collision and this changes to k prime, k 1 prime after pollution and this integral is over the wave vector space you have d k, k 1 k prime and k 1 prime .

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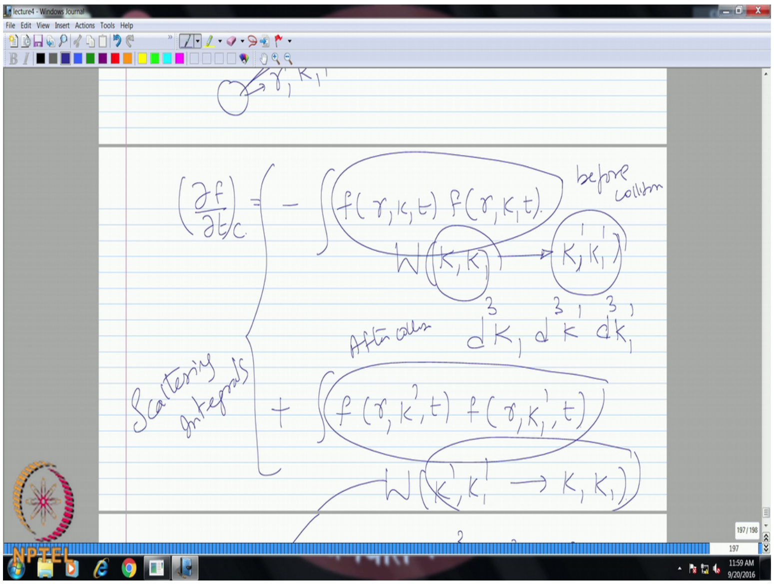

Now this is a very complex integral, you have to integrate it is integrate this over d cube k 1 and d cube k prime d cube means here, we have three dimensions we have k x k y k z and not only that. So, this becomes therefore, triple integral in terms of k triple integral in terms of k prime. So, this is k prime is after collision and then another triple integral for the second particle after collision, this is one such integral and you have again another integral we which will be f r comma k prime.

So, this is your first particle after the collision time's f r k 1 prime t. So, this you can consider is the distribution before collision. So, this is here before coalition term and this is your after collision. The rate of change in the scattering is what we say after collision minus before collision. So, that is how we are writing. So, this again you have the function which goes from k prime k one prime to k, k 1 and again you have the integrals 3 triple integrals.

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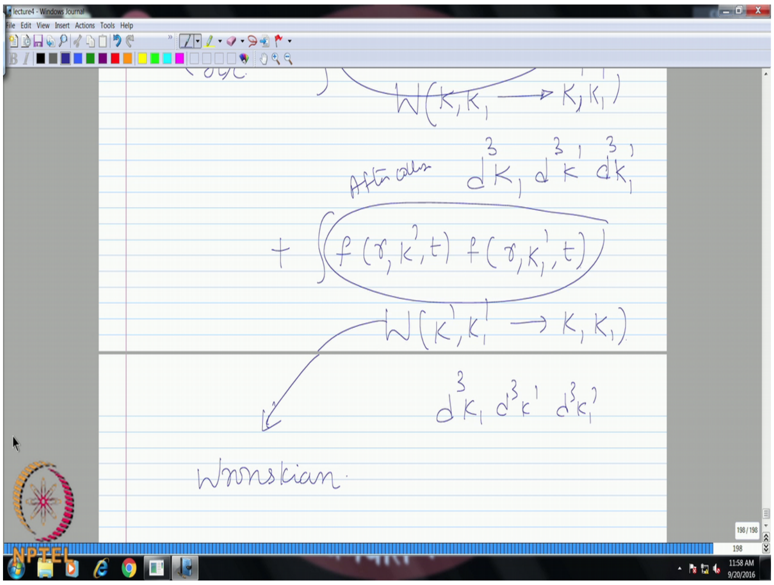

So, totally it is actually 9 integral we have k 1, d cube k prime, d cube k 1 prime, where this w function is called wrong scale functions. So, I am not giving all the details, but this is called the Wronskian, and this particular function in this case will be giving you a function to tell you what will be the change in the wave vector, from an initial wave vector for example, in this case this is pre collision and how it is related to the post collision and similarly here post collision.

So, you have due to the coalition certain number of particles with a wave vector k k 1 changing to a wave vector k prime k 1 prime. So, this is going out. So, this is out going out from, out scattering, out from a certain wave vector space there is another distribution here, which is coming in from another wave vector space k prime k 1 prime to this value of k and k 1.

So, what we call as the simplest possible collision between two particles this is represented by a very complex scattering integral. So, as you can see those these are all integrals and in collection they are called the scattering integrals. So, you are talking about therefore, 9 integrals here correct. So, therefore, this again computationally people have never attempted to solve this; that means, you have to keep track of the wave vector before collision, after collision for each particle and then you are now talking about calculating 9 integrals and therefore, this gives you the coalition between just two particles again the more complex scattering integrals are therefore, three particle collisions and so, on.

But, why I want to emphasize this just to understand the sheer level of complexity when you deal with the simplest possible collision. So, this is a computationally prove prohibitive task to calculate the collision terms even for a two particle system therefore, a huge simplification of this is made. So, we will talk about that in the next class tomorrow so, but what I want to say is look at the levels of simplification that fitted starting from a capital n number of particles to one particle and again the collision is now completely approximated to something very, very simple, but still the resulting equation is still called the Boltzmann transport equation with a relaxation time approximation.

So, the original Boltzmann transport equation is this one with a very complex scattering integral. However, to solve this practically we use the replace the scattering integral with what we call as relaxation time approximation. So, that is what is generally salt to describe the transport from we will stop here.

Thank you.