Micro and Nanoscale Energy Transport
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Lecture – 13
Fundamentals of Solid State Physics Part 2

Say very good morning all of you. In the last class we looked at the energy bands in solids and the energy bands which are coming out from solving the Schrodinger's equation for the entire crystal. That means, we have taken one dimensional structure of atoms capital a number of atoms and then we saw I mean solving Schrodinger's equation how we can produce the discrete values for the a wave vector K and also there is another wave vector coming from the entire crystal that is the small K and then we saw that now this small K will lead to quasi continuous values of energy that is one thing the other is when we solve the particular Schrodinger's equation you have to satisfy the condition that you know you have a cos times the wave vector for the entire crystal times the lattice spacing a.

So, based on this we find that there are solutions which are not allowable and these form you know discrete bands where you know. So, these are basically the reason why we have the energy gaps between the different energy states or energy levels in you know different materials such as metals, semiconductors, insulators and so on. So, the electrons have to fill within these energy levels and also account for the discontinuities in the energy levels through these kinds of jumps or band gaps.

So, depending on this concept of band gap; so the band gap is inevitably going to be there; so, but the classification of these materials will now depend on the way the electrons are filling these. So, in the case of metals; the electrons will be you know; not completely filling a particular energy level.

Therefore, they are free to move and this becomes the conduction band whereas in the case of insulators; the conduction band is completely filled there is no room for the electron to move around in that energy level and also the fact that you have a very big band gap. So, they cannot even jump from one band to the other. So, these pictures whatever I have drawn they were all at respect to zero Kelvin filling of electrons that is the default state of that material at lowest energy level possible.

Now, if you are exciting this at much higher temperatures these electrons tend to move around to the higher energy states and for example, the picture of an intrinsic semiconductor; that means, that at a finite temperature; so they can overcome the band gap or the energy required to jump from one band to the other and therefore, they become conducting material whereas, at zero Kelvin they look like semiconductors whereas, at some temperature they become a conductor whereas, if you are looking at extrinsic semiconductors I mean the band gap is little too higher.

So, even at you know normal temperatures like room temperature and above they cannot jump across the band gap so easily and therefore, you need an external material whose Fermi level can basically adjust either between the valance or the conduction band of this particular semiconductor material. So, the external material can be either a donor or acceptor depending on where the Fermi level matches with this base material; base materials conduction band.

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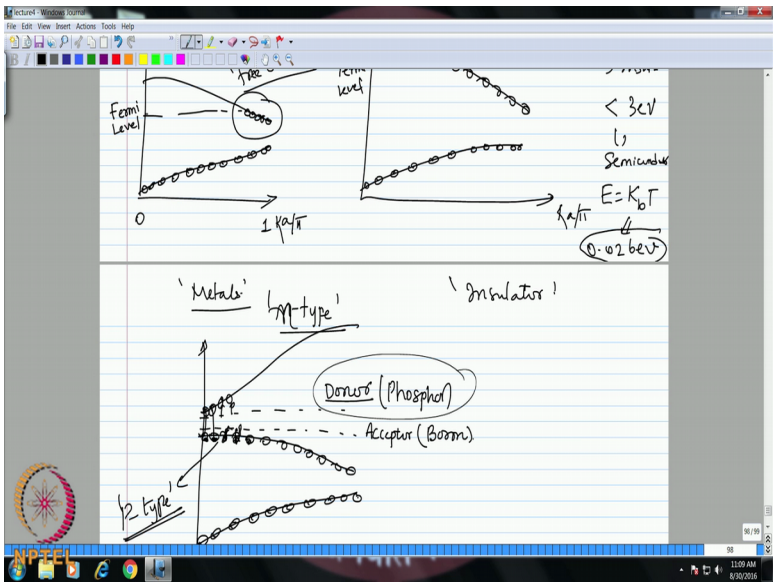

So, if it is too close to the conduction band; so we have called this has the donor. So, some electrons from the donor get excited and they get move to the conduction band of the base material. And therefore, now the electrons are abundantly available in the conduction band to move around then this becomes n type semiconductor. So, whereas, if you talk about acceptor material. So, the Fermi level of the acceptor material will be close to the valance band and therefore, some of the electrons from the base material

jump to the acceptor material thereby creating some empty spaces and therefore, again in the base material you have some room for the electrons to move. So, this becomes the absence of electrons these are called now holes there is nothing physically called holes this only the absence of electrons it means there is just more rooms. So, this kind of semiconductor material is called the p type semiconductor material.

So, from the quantum mechanical perspective; we are now able to understand why there is an energy gap that is arising and how as a consequence of this energy gap and depending on the filling of the electrons you can end up in classifying different materials right. So, this is a very very important step you know before you proceed further in analyzing the energy transport; in these materials you have to first know their classification. So, what we will do now is just in the last class we have drawn these kinds of energy bands which actually look like this, but we will only now focus on the valance and conduction bands.

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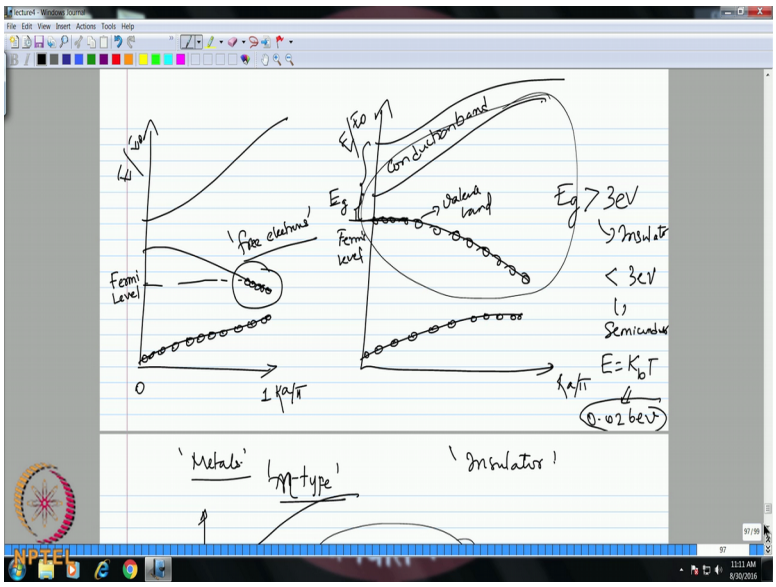

That is we have seen that in all these cases; so we are mostly concerned with the movement of electrons in these two particular bands right. So, it can be either completely filled or partly filled or it can jump from this band to that band. So, never the less these two are the bands of interest. So, the lower one is the valance band the upper one is the conduction band in case of you know p type semiconductor even the lower one can become the conduction band, but in general now if you take a generic material.

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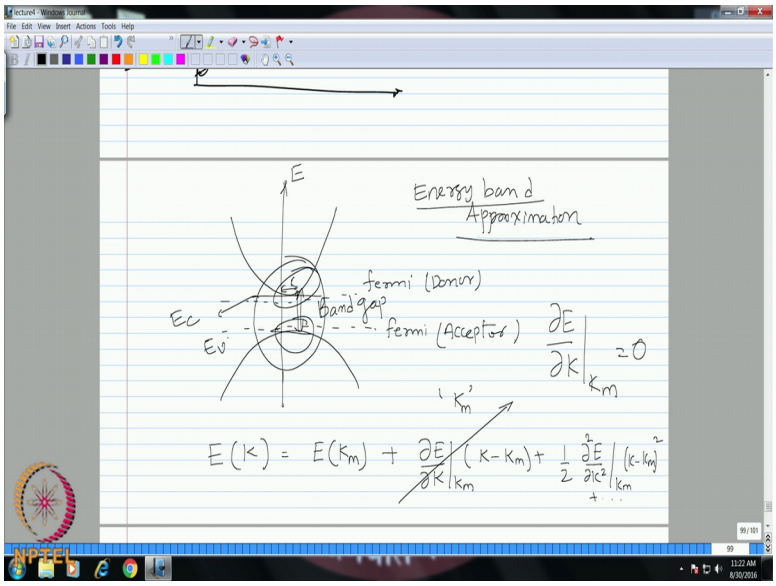

So, we will focus only on these two bands. So, therefore, we will approximate these bands by again a parabola right.

Essentially, the lower band of this is represented with one parabola, the other one with another parabola. So, we will end up having two parabolas like this, inverted and then you have the band gap this is your band gap. So, this is approximation to the real energy bands. So, you can call this is energy band approximation. So, this is easier to work with if you want do some theoretical analysis.

So, why we are doing this way is that now if you draw the energy on the vertical axis right and now if you are talking about n or p types. So, now, in the n type semiconductor the donor will have a Fermi level which is closer to the second band the upper band in the case of the p type the acceptor would have a Fermi level which is closer to the lower band right. So, these are the impurities what you call you know the donor or acceptor. So, for the base material you are adding certain impurity and you are doping it.

With this case what we can do is use a Taylor series approximation because now according to this analysis this is the symmetric one. So, that is why we can draw only one half; either the right or left one we have represented only one half in the earlier figures, but actually as you can see from the original graphs they are symmetric; they can stretch from now values of the crystal wave vector spanning from minus pi by a to plus pi by a right. So, they are therefore, symmetric, but you can therefore, see that the

movement of these electrons are mostly confined towards either the maxima of the lower band or the minima of the upper band.

Most of the materials you know unless they are excellent conductors or very bad insulators where you do not have any movement at all or excellent conductor where it may be filled all the way till here may be sometimes and you have a lot of space again, but most of the semiconductor materials for example, will have most of the movement of the electrons taking place between the maxima of the lower band and the minima of the upper band.

Therefore, we will only focus on this particular region and then apply Taylor series approximation to calculate the energy level at some wave vector; some displaced wave vector from the center at which you have the maxima or minima. First of all we do not know whether the maxima or minima is at the center. It could be slightly offset from the center axis also. So, let us say that the location where you have either the maxima or minima for the wave vector this basically K m and therefore, if you use the Taylor series approximation you can calculate the energy corresponding to some vicinity of this K m and some other value K which is related to the energy at K m plus what; how do you expand in the Taylor series we have therefore, derivative of this at K m times K minus K m plus you have half of d square E by d K square at K m into K minus K m square plus higher order terms. So, this is the Taylor series to the second order approximation.

So, now we can. Therefore, write this now we know that at the maxima or minima point what is the condition that we can apply. So, we have d E by d K at K m will be zero. So, we are now concerned only about the region where we have the maxima or minima. So, where we are using the Taylor series or the points where you have the inflection point. So, this condition zero this should be equal to 0.

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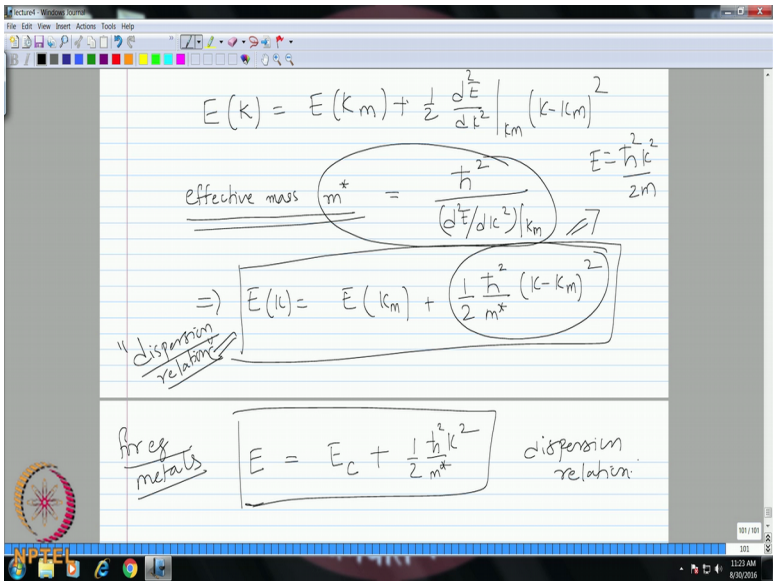

And therefore; so, now, we are making a simpler approximation to these energy bands this is K m plus half d square E by d K square; now I am going to introduce another notation here this is called as the effective mass at I use the symbol m superscript star to distinguish it from mass of a particle mass of a particle like electron mass, phonon mass or whatever they are just m subscript e or whatever in the Schrodinger's equation.

Now, I am using another notation m star. So, I am going to define this has modified Planck's constants square divided by d square E by d K square; this derivative evaluated at the saddle point. Therefore, if you use this definition you can rewrite these d square E by d K square as what h prime square by m star. Now, therefore, we are rewriting this in the form which is little bit more familiar the relationship between energy and wave vector that we get in Schrodinger's equation.

Now, we are going to rewrite it in the similar format by therefore, we have m star write into K minus K m the whole square. So, now, you see this and compare it to the energy from Schrodinger's equation; how it is related to the wave vectors. So, there how did we relate it? h prime square K square by 2 m. So now, we have brought it to the similar format here except that now instead of mass of the particle you have the effective mass m star. So, this m star is kind of representative of the crystal mass; it is not you cannot call this as anything to do with mass of a particle here because this is not real mass; it is some kind of the units of this will come to mass, but it is to do with the crystal energy bands.

So, therefore, this is actually representative of the crystal mass not the physical mass it is actually a some kind of mathematical representation.

So, this is basically the relationship between the energy and the wave vector k; this K is a small K this is for the crystal wave vector. So, this is your dispersion relation for the entire crystal. So, we have therefore, using this parabolic approximation and now we have applied the Taylor series and we have come to this; we can use it for different materials and we can actually rewrite this in terms of conduct; for example, if your applying these to the conduction band. So, the corresponding energy will be equal to the point where you have the minima for the conduction bands. So, this you are starting of the conduction band. So, that is this point; this point is the starting of your conduction band this is the point where your valance band ends.

So therefore, if you are applying this to the conduction band where suppose you are talking about metals; so your conduction band is partly filled. So, in that case starting point will be the minima of the conduction band plus you have half h bar square by m star and now you can also assume that it is symmetric about the central line. So, the point where you have the minima is K m equal to 0. Therefore, this becomes much easier to approximate.

For example, you can talk about metals. So, this is the dispersion relation between the energy and wave vector. So therefore, if you are just to summarize the transition from the simple systems in quantum mechanics to a real structure.

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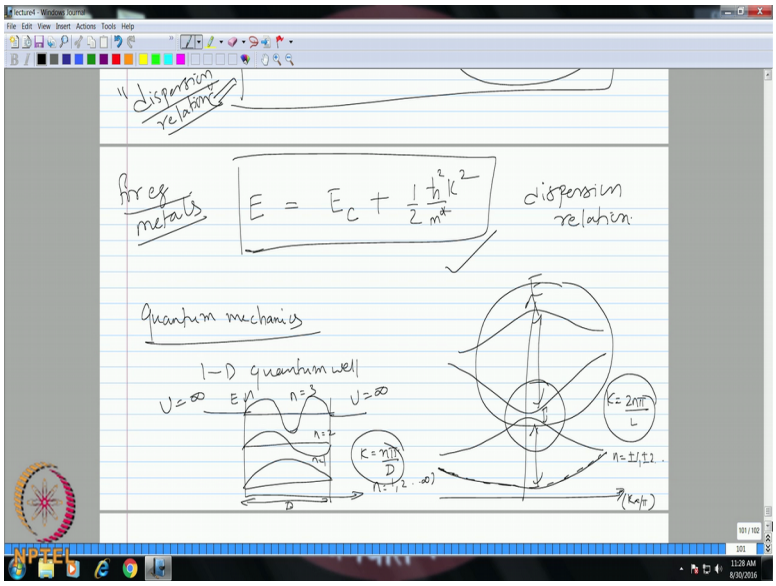

So, in the case of quantum mechanics of simple systems; let us say quantum well. You have basically the 1-D quantum well in which how was the dispersion or how was the structure of the energy levels? So, you had quantum well like this and then you had width of say D and on the vertical axis you have the energy. So, this cannot escape the potential energy constraint outside say U equal to infinity. So, in this case you had different modes.

So, your energy levels were all quantized. So, it defined by the jump in the wave number or wave vector. So, K equal to n pi by D. So, you have n equal to 1; you have particular wave function and corresponding value of energy and for n equal to 2; you had a particular wave number corresponding value number of energy and n equal to 3; n equal to 2; this n equal to 2 and n equal to 3 and so on. So therefore, so you had your discretization of the wave number where n equal to 1, 2 and so on. So, correspondingly your energy level where also discontinuous and they were quantized.

Now, in the case of a crystal structure; when you are looking at quantization; now two levels of quantization are there. One; your K is quantized in a crystal; how was this related? 2 n pi by L. You have seen this in the case of crystals where n can take the values plus or minus 1 plus or minus 2 and so on. So, this is one level of quantization and the other is due to the solution of the Schrodinger's equation and the solution which says that there are non allowable solutions and therefore, there are band gaps.

So, the consequence of applying the quantum mechanics to a crystal now is on top of this discreteness in the wave vector space; also you have jumps between the energy levels resulting in the band gaps. So, therefore, you ended up with; so, you had a particular band; so in ffact, these were all discrete. This is what I meant by your plotting this with for example, K a by pi. So, I want this concept to be very clear. So, that you do not get confused.

So, this discreteness here in small K results in these quasi continuous bands here. These are not perfectly continuous here; just discrete, but we are representing it like this. Now these are equivalent to these jumps. On top of this you also have gaps between the energy levels therefore, the next level would be looking like this and then you have the next energy level like this, you have the next energy level like this ok.

So, in the crystal structure therefore, you have one level of discontinuity because of this K and also the other level of discontinuity due to this band gaps. So, this is your real dispersion curve and then we made an approximation to these bands; these two bands for example, and then we have arrived at this particular dispersion relation here. Is it clear?

So, what we will do next is now we; so far we focused on the electrons. So, the electrons confined by a certain potential energy constraints due to the interaction of atoms in a crystal. So, we will now move on to what will happen to the Vibrational energy of these atoms. So, in actual crystal; now we also look at the simple harmonic motion. For a single atom we looked at spring mass system equivalent and then we derived the quantum mechanical energy states h nu into n plus half right. So, n can go from zero all the way. Now, if you expand this to a crystal with n number of atoms. So, how is this interaction between atoms going to be accounted in this harmonic motion? So, this will be the next.

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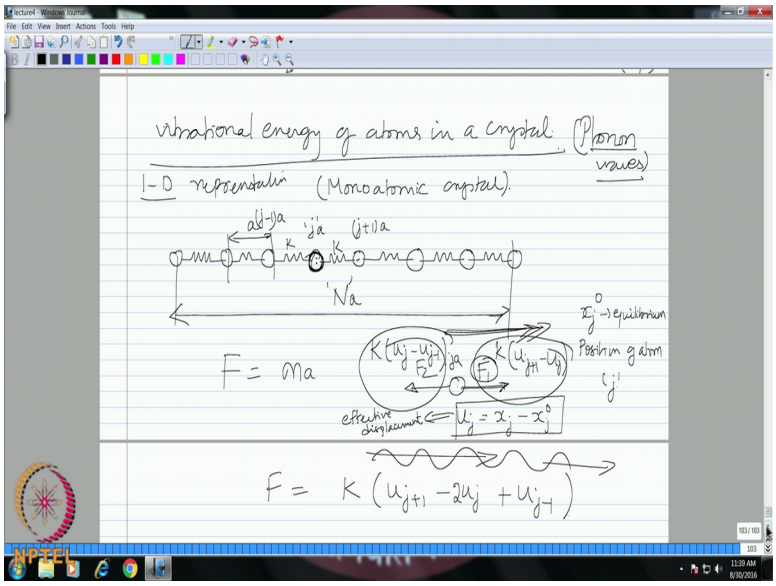

So, basically you have the vibration of atoms; Vibrational energy of atoms in a crystal. So, we are going from quantum mechanics of simple system to now more complex systems we did for this for electrons now next will do this per phonons; that means these are what? Phonon waves right. Once again we have analyzed a single particle Vibrational energy state before. So, mow we will do this collectively for many numbers of atoms together. So, these will be the actual Vibrational waves are termed as fictitious particles called phonons.

So, therefore, we will construct a simple model for analysis. See there are many ways of looking at this you can actually solve the Schrodinger's equation again, but we will now resort to a more common and simpler way of handling this collective Vibrational energy of the atoms. So, unlike the electron case where we were more rigorous, we knew the potential energy constraint and solve the Schrodinger's equation; here we will use some classical mechanics, some kind of conversion to the wave nature and then we will bring in whatever you have already derived in the quantum mechanics for a Vibrational energy and plug it into this. So, we are going to do some little bit of ad hoc approach here, but that is probably the easier way to deal this problem.

You can imagine the interaction between all these atoms together as several masses connected by springs. So, you have one atom described by this particular mass, neighbouring atom and the interaction between them through a spring constant. So, we

will consider only simple harmonic motion like this back and forth. So, like this you have several of these atoms in a crystal. So, all connected by this same spring with same spring constant and the separation between them can be denoted as a. So, you have n number of atoms forming a crystal. So, this is just a one dimensional representation. We are talking about 1-D representation; the actual crystal is three dimensional. So, we will also have in the vertical direction into their depth, but we will decouple all of them we will not say this motion is going to influence vertical motions. So, we will have decoupled things and later on we can linearly to superpose those solutions.

So, first we will therefore, look at only the 1-D representation; so the total length of this 1-D chain of atom. So, these are basically monatomic crystal. You understand. So, you have basically only one kind of atom in the crystal and there all just equidistant spaced and they are separated; you can also have a polyatomic structure, you can have two atoms one bigger size one smaller size with different masses, but right now to start with we will look at simpler system.

The total length of this chain therefore, will be N times a where N is the number of atoms. So, the particular coordinate of an atom; so here for example, this atom we will call this as j times a where is an index. For example, if this is the fourth atom from the left. So, this will be number 4; and therefore, this will be j plus one 1times a; and this will be j minus 1 times a. So, these are the actual coordinates. I am using this index notion here because you can apply this to any of these atoms. This will be collection of so many numbers of atoms that practically it will not make a difference if you use N or N plus 1. If you are talking about 10 power 26, 10 power 28; number of atoms so it will not make any difference of you add 1 to that. So, we can just make it as N a.

Therefore, what we will do now is go back to classical mechanics. This is where we will do some little bit of cheating; we will not follow the regard that we did for electrons; we will just use the Newtonian mechanics here; F is equal to m a. So that means, we will consider a particular atom here at location j a; and look about the forces acting on this particular atom. So, you have one force acting in this way, the other force which is acting in this way. So, there is a pull coming from here, pull coming from here. So, therefore, the effective force will be the difference between these two forces.

Now can you write down what will be the force acting on this direction; that means, between let us only consider neighbours now; let us not complicate it by including a very large neighbourhood just immediate neighbour. So, that is the force between this atom and this atom. So, we know the spring constant k. So, I want you to just write down the forces. Now let us also I will give you some nomenclature here; let us say that the equilibrium position of this atom to begin with is x j superscript zero. This is your equilibrium; equilibrium position of atom j a; at location j a.

So, now if you are pulling; now from this equilibrium position there is a certain displacement. So, therefore, the actual displacement from this equilibrium position will be; let us say will use this notion u j; this is not velocity here this is you are effective displacement from the equilibrium. So, your new location would be something like x j minus your original location x j. So, this u j is actually the effective displacement from the equilibrium position.

Therefore, knowing the displacement of this atom j and similarly you will know the displacement of the atom j plus 1. So, you can calculate the force which is acting this direction first between the atom j and j plus. So can you express this; you also know the spring constant and then similarly write it for the other force. So, what will be the force? How can we write it? Spring constant times.

Student: (Refer Time: 32:57).

U j plus 1 minus u j. So, U is the effective displacement from the equilibrium. So, we will use U not x right. Similarly; you are right. This is equivalent to x j plus 1 minus x j, but we will write in terms of U. Similarly in case of F2; K times u j minus u j minus 1. So, therefore, the net force will be the difference between this and this right. So, the net force which is acting in this direction; which is pulling the particular atom j to the right will be this force minus this.

Now what will happen in the in the wave nature now this will produce a right running way effectively in this direction right. Therefore, the net force will be K time's u j plus 1 minus u j minus so you have 2 u j plus u j minus 1. So, this is the net force acting in this direction in terms of wave picture it will now produce right running wave which is moving in this direction; this Vibrational energy.

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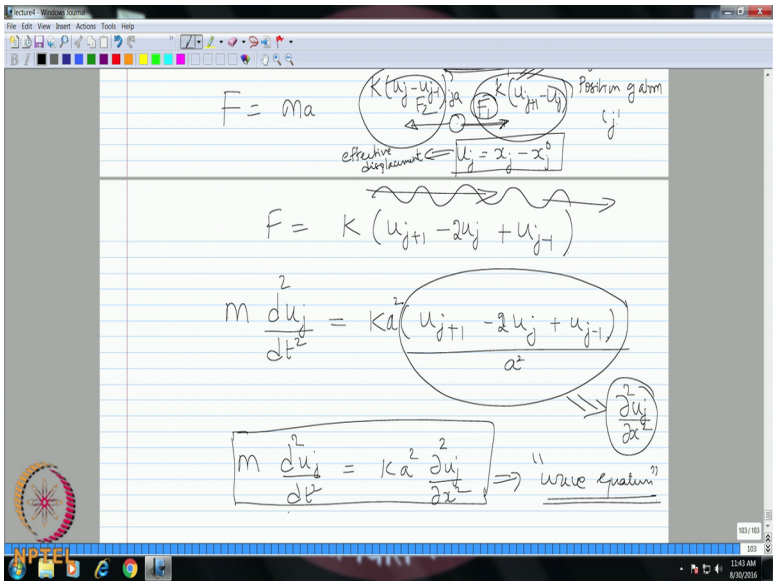

Therefore, now going back to the classical mechanics m into d square what should I write here? U j by d t square; this is the acceleration of this particular atom in the right direction; this is equal to K time's u j plus 1. So, I can multiply and divide it by a square where a square is the lattice spacing between the atoms. So therefore, now what do I see here anybody who has done numerical methods. So, this is the central difference form of what? What is the operator? Student: (Refer Time: 35:22) d square u j by Student: (Refer Time: 35:27) d x square.

This is the numerical approximation now because we are working with discrete spaces; because lattice is what? What is a crystal? Crystal is nothing, but atoms which are located in discrete points in space. So, what we can get here is only a discrete representation; if you want to transform this into a continuous derivative so you have to imagine like you apply a numerical approximation to continuous derivative and then you back transform that. Therefore, if you want to write this in terms of continuous equation so therefore you have m d square u j by d t square will be equal to K a square into d square u j by d x square. So, what kind of equation is this?

Student: (Refer Time: 36:29)

Correct, but now we are writing this in terms of space. So, to distinguish this so we will have u j which is now functions of both space and time. So, therefore, we have converted that into partial (Refer Time: 36:53). So, what type of equation is this? (Refer Time:

36:59), mathematical, parabolic, elliptic or hyperbolic? Why elliptic? Student: (Refer Time: 37:10) How many of you say hyperbolic? So, this is basically hyperbolic equation. This is your wave equation.

People who are done some differential equations; you must a studied; this is your wave equation and wave equation is always hyperbolic. This d square u by d t square will make all the difference. If it was just d u by d t this would have been parabolic equation. So, this is your hyperbolic wave equation; this is your also called your telegraphic equation whatever these are basically all these are waves. To describe the waves so this is your commonly used wave equation.

So, you have displacement of a string that you study in your partial differential equation. That is basically governed by these equations from some equilibrium position you displace the string and you have waves. Now you want to study the how these waves are propagating from the initial condition. So, solve this p d a for that.

Coming back to this problem, what we have is we are trying to find a solution to a discrete problem. We are trying to find a continuous solution to a discrete problem. So, we are discretized already points in space and now we have transformed this into a continuous equation here. So, how will the discontinuity be addressed in this continuous solution? So, we will see that. So, now, what it means; you have a wave therefore, which is propagating, but in which direction it is propagating effectively towards the right.

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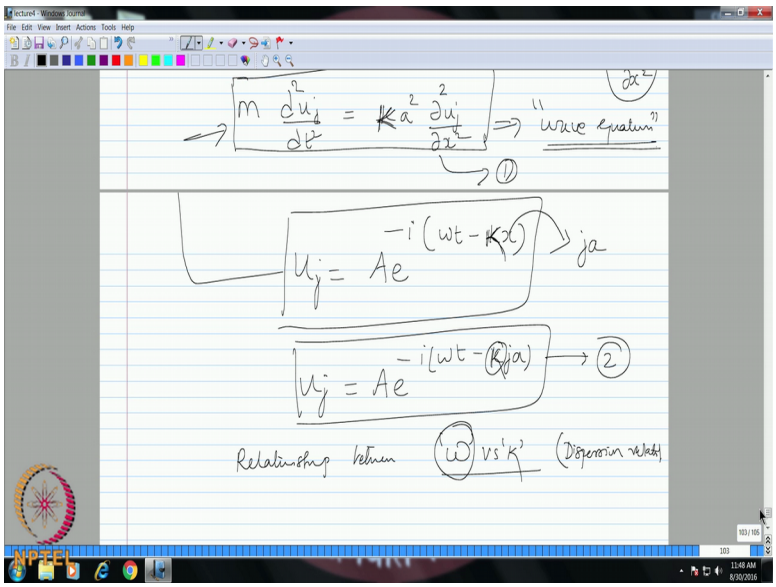

So, the solution to this will be a right running wave. So, which will be A e power minus i omega t minus K x. So, this is your solution to this equation. Now this is a continuous solution, but we have discrete set of points. So therefore, how do we transform these? We just plug in for x as what? X is continuous. Now, we will use j times a. Therefore, for this particular problem you have A e power minus i omega t minus K j a. This becomes a discrete solution at each and every location j you will find the correspondent.

So, what you can do substitute this solution into let us say this is equation 1 and this is your assume solution for the wave equation; substitute this 2 into 1. This should eventually satisfy this and you write down the relation between; now omega what we have is your angular frequency here. So, this omega and we want to construct relationship between k; this K here. Now let me not put this into; so this is your k. We are using only one K here. Now this K is your spring constant. I think let us use kappa here; this kappa is your wave vector.

Student: (Refer Time: 41:10).

What is that?

Student: (Refer Time: 41:13).

So, you use I mean whatever notation you want, but this is your spring constant here and this will be your wave vector kappa; you can denote it like this. So, you substitute this into this equation write down therefore, relationship between omega; this is also your kappa. So, write down relationship between the angular frequency omega and kappa. So, this is what is this relation called dispersion relation.

In the case of electrons you used energy e verses the wave vector. So, in the case of phonons; the energy is now denoted by the angular frequency omega. How it is related? h bar omega. So, therefore, now we are having dispersion relation for phonons between omega and kappa. So, can you do that? I will give you five minutes time. I think you should be able to do this. Student: (Refer Time: 43:23) K a square; this is your final relation you are getting? First find d u by d t; then you find d square u by d t square and then you substitute.

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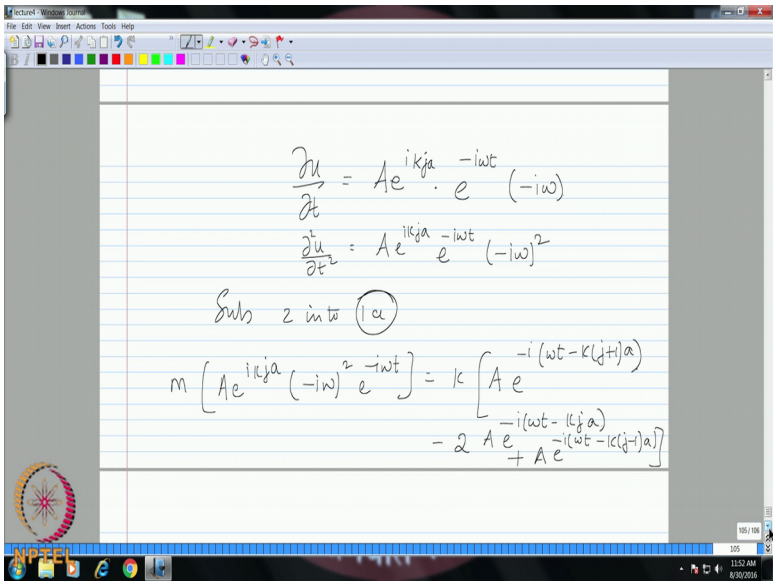

First find out d u by d t. So, what do you get d u by d t? So, A e I; you will have A e I K. So, let me separate this special part out. So, then you have e minus i omega t into minus i omega. Then you do d square u by d t square. So, now, this is again a constant you will not and now this will be again e for minus i omega t. So, this will be minus i omega the whole square. So now, their time derivative is determined. So, similarly find out the special derivatives.

Student: (Refer Time: 45:11).

No, it is not that simple; you will have a trigonometric function there. You should have a sine function on the right hand side in terms of kappa. So, what you can do now; is you can substitute this to in fact, to make it easier you can you can substitute; let me call this as equation 1 a; because this is a discrete one and this is also discrete solution 2. So, directly this 2 can be substituted into 1 a. Then the right hand side part becomes discrete. So, do not have to worry about it. Therefore, substitute 2 into 1 which is the discrete equation.

So, I will just write down m A e power i this is the temporal part; minus i omega square e power minus i omega t. So, now, the right hand side is already discrete you just plug in for the appropriate index; i omega t minus K what do you have j plus 1 a. T his is u of j plus 1 minus 2 times u of j this is A e power minus I omega t minus K j a plus you have u of j plus 1; j u of j minus 1 e power minus I omega t minus K j minus 1 a.

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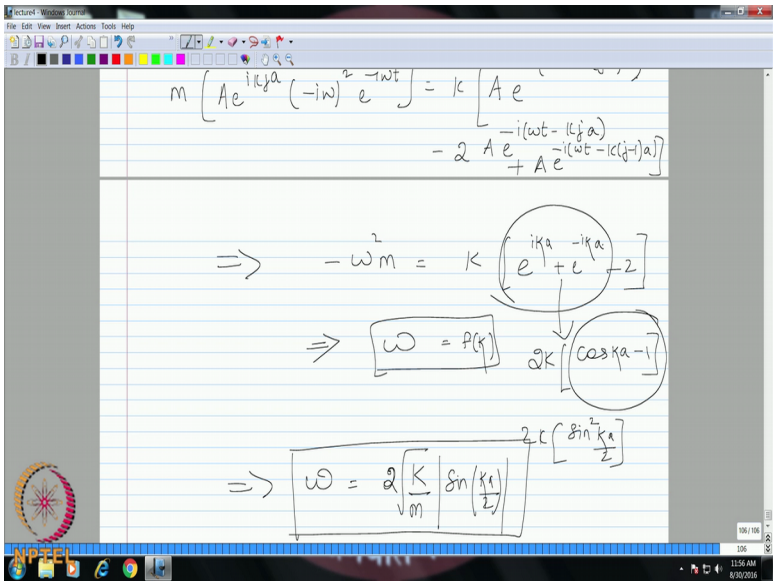


Now if you cancel all the common terms you will be getting minus omega square m is equal to K and e power I this is your kappa plus e power minus I kappa a minus 2. You can actually pull e power minus i omega t out and cancel of left and right because they are common and this is what you will get. Now you use the relationship between this and your trigonometric functions.

So, tomorrow you tell me how will you convert this into trigonometric function therefore, form that what would be the relationship between omega and kappa. Please do these as a home work from there will continue and one thing you might remember the relationship between this directly and the trigonometric functions. So, what will this be?

Student (Refer Time: 48:50).

Two times; we have cos K a minus. So, we have 2 common. So, this will be minus 1. So, therefore, how can write this again, 1 minus cos K a minus 1. So, this should. So, this should come out to be sine square.

Student: (Refer Time: 49:31).

We can use the half angle formula; half angle trigonometric identity kappa a by 2. So, therefore, your omega can be written as 2 times square root of. So, omega can be positive only because it is like energy, so it cannot take negative values. So, this is your spring

constant here and you have absolute value of sine kappa a by 2. This turns out to be the dispersion relation.

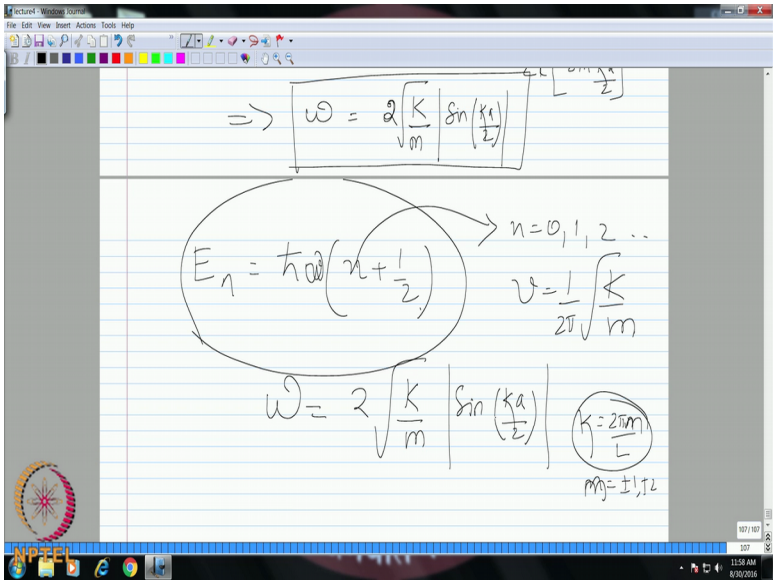
Student: (Refer Time: 50:20).

Where?

Student: (Refer Time: 50:23).

This is half angle formula. This is not simply 1 minus cos square is equal to sine square theta. This we are using the half angle formula; you please check that. All these we have derived by classical mechanics. Now, how are we going to apply quantum mechanics to this? Now remember our energy levels for vibration.

(Refer Slide Time: 51:03)



So, we have derived E n is h nu n plus half right or we can write this as h bar omega h by 2 pi into 2 pi h by 2 pi is h bar h bar times omega. Now there we had relationship of nu as 1 by 2 pi square root of K by m in the spring mass system in the simple harmonic oscillation. So, now, this omega is now become what discrete. 2 times square root of K by m. So, similar, but you have absolute value of sine kappa a by 2; now your kappa is what 2 pi n by L where n is plus or minus 1 plus or minus 2 now this is become discrete and therefore, your omega is become now discrete. Now this is how for the actual crystal your energy levels have become discrete.

Again you have two levels of discreteness. One is your n here; maybe you can use m here to distinguish that n an m. So, your n here is one level of quantization which is taking values from 0, 1, 2 and so on. The other discreteness in your value of angular frequency omega which is now functions of the wave vector which is again now discrete. So, just like your electron energy levels. Now you have again discreteness not only in the modes, but also in the energy levels energy bands.

This is how we are now dealing with the phonon energy level. So, we have really not solved the Schrodinger's equation fully; we have assumed the same energy vibration energy levels or energy whatever we have derived before should hold true for this system except for the fact that now omega is now modified through this dispersion relation. So, we will stop here and tomorrow we will continue what is the consequence of this.

Thank you.