Introduction to Solid State Physics
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Lecture - 50
Density of states of Phonons

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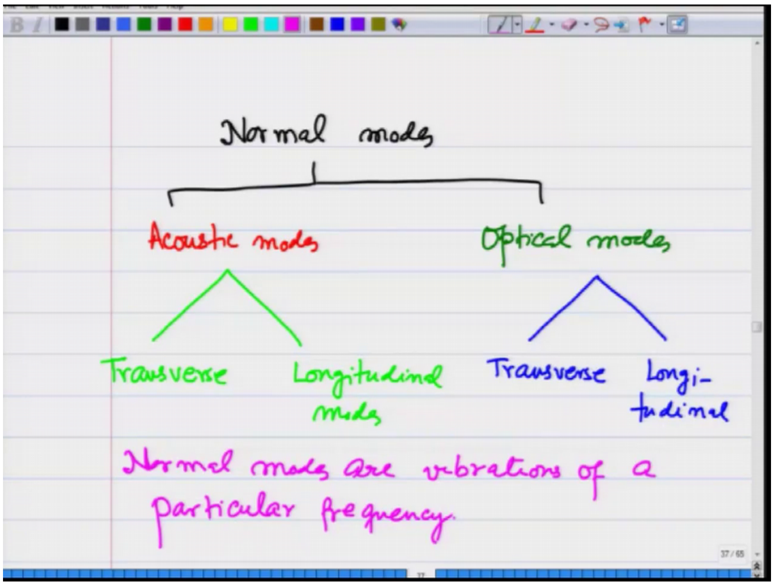

Normal modes are vibrations of a particular frequency.

So far I have shown you that the atoms in a crystal vibrate and they create something called the normal modes. These are two kinds, acoustic modes and optical modes. And again in these I can have transverse and longitudinal modes. Same thing in the optical modes, I can have either the transverse or longitudinal modes. So, this we have worked out. Now, what normal modes are? So, normal modes are vibrations of a particular frequency.

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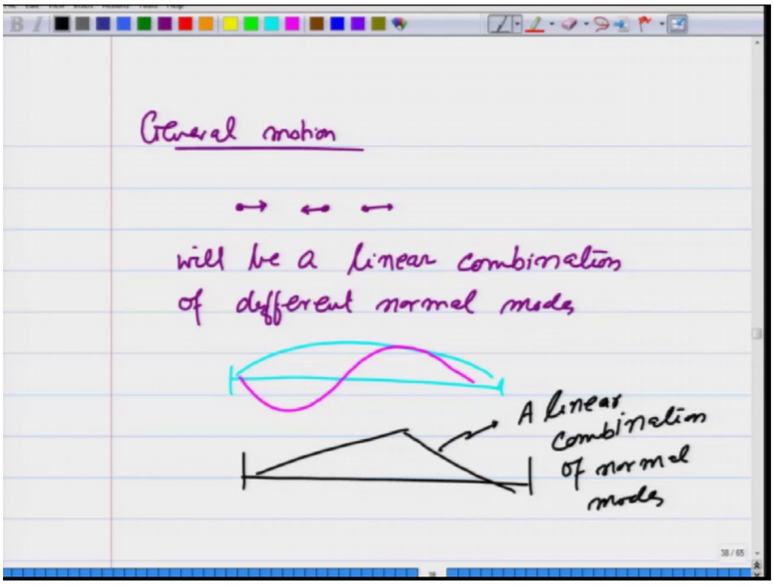

General motion

will be a linear combination of different normal modes

A linear combination of normal modes

And if I want to describe in general motion; a general motion of a lattice that means, one atom could be moving like this, one atom could be moving like this and so on and need not be like a wave, then general motion will be a linear combination of different normal modes. Just like if I have a string; its normal modes are the vibrations of given frequency like this. But, if I give a general displacement to the string, let us say like this, this is a linear combination of normal modes. So, this is what we have covered so far.

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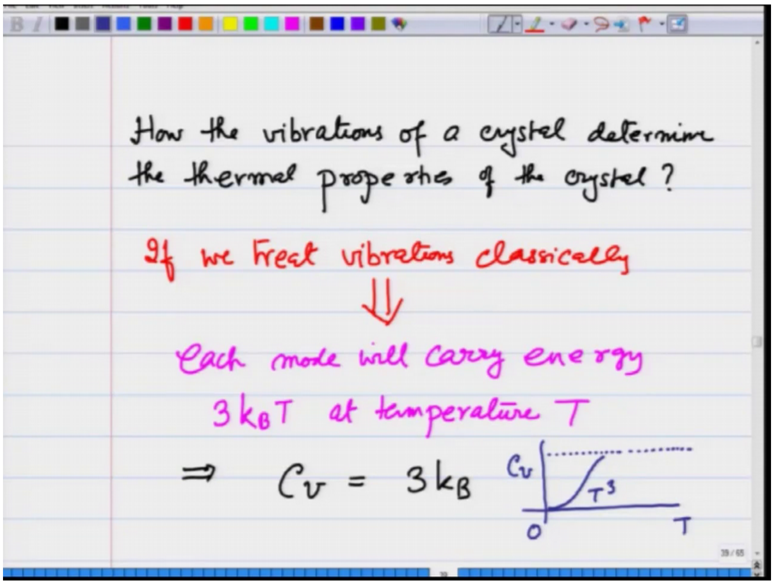

How the vibrations of a crystal determine the thermal properties of the crystal?

If we treat vibrations classically

$$\Downarrow$$

Each mode will carry energy $3k_BT$ at temperature T

$$\Rightarrow \quad C_v = 3k_B$$

With this background, we are now ready to understand how these modes affect the thermal properties of a crystal. So, what we are going to study now, how the vibrations of a crystal determine the thermal properties of crystal? Because, after all what are vibrations, vibrations are atoms moving around and these carry energy. And these energies are given by the thermal energy in the background. So, thermal properties are determined by these vibrations.

Let me just recall that in the previous part of this course, Professor Satyajit Banerjee derived the specific heat of electrons and mentioned that the ions in the background give a different kind of specific heat. In particular, what he said was that the specific heat of conducting electrons goes as linearly as T for low temperatures, whereas the specific heat of background ions due to vibrations goes as T cube. And this is what I am going to show you, how it comes about.

Now, I had also told you earlier that experimentally it is found that the vibration should be treated in a quantum mechanical manner. Let me now come back to it and show why it should happen. If we treat vibrations classically, then this implies that each mode will carry energy 3 k B T, where k B is the Boltzmann constant and T is the temperature at temperature T. It is not 3 by 2 k T, but 3 k B T, because there are two quadratic terms in the energy. One the kinetic energy term, and the potential energy term and both are 3 by 2 k T.

And this immediately implies that C v is going to be 3 k B. And experimentally, this is not found to be the case. If I were to plot the specific heat, let us show it schematically here. As a function of temperature C v, according to this what is known as the due long period law, it should be a constant 3 k B T like this as a function of the temperature.

But, insulators you find that it goes as T cubed at low temperatures. And that is it goes as T cube and goes to 0 in particular at 0 temperature. And that is explained only if you treat vibrations quantum mechanically, so it is absolutely essential that the energy of the vibrations be treated quantum mechanically and that means, the energy of vibrations be treated as the energy of a harmonic oscillator in the quantum mechanical sense.

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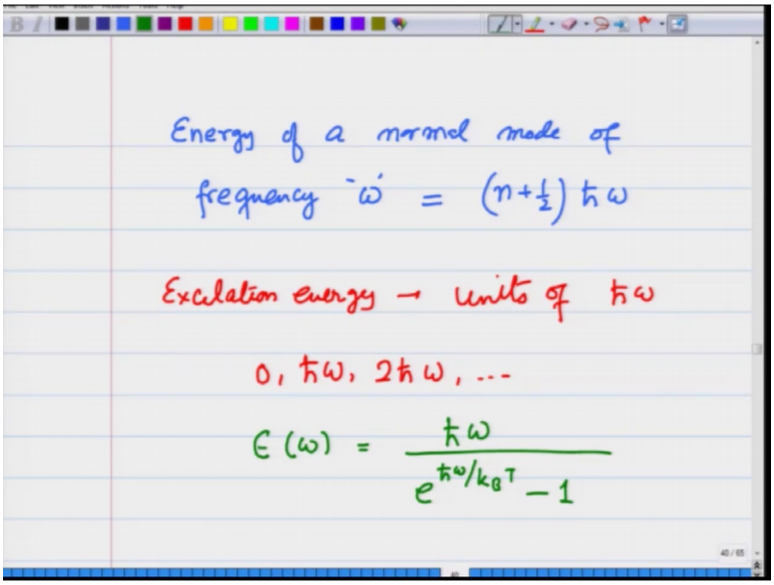

Energy of a normal mode of frequency ω = $(n+\frac{1}{2})\hbar\omega$

Excitation energy → units of $\hbar\omega$

$0, \hbar\omega, 2\hbar\omega, \ldots$

$$\epsilon(\omega) = \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$$

So, what we understand is that energy of a normal mode of frequency omega will be given as n plus half h cross omega, which is the energy of harmonic oscillator. In particular, what we will be focusing on the excitation energy and this comes in units of h cross omega, because I will ignore the ground state energy half h cross omega for that. So, the excitation energy is either 0, h cross omega, 2 h cross omega and so on.

So, now we pretty much know what the energy of the system is going to look like. And at temperature T the average energy of an oscillator at frequency omega is given by Planck's formula and this comes out to be h cross omega over e raised to h cross omega by k B T minus 1, this I will derive a later also, but right now let me just mention this. So, as far as the energetics are concerned, we know all about what the energies of these normal modes are and everything.

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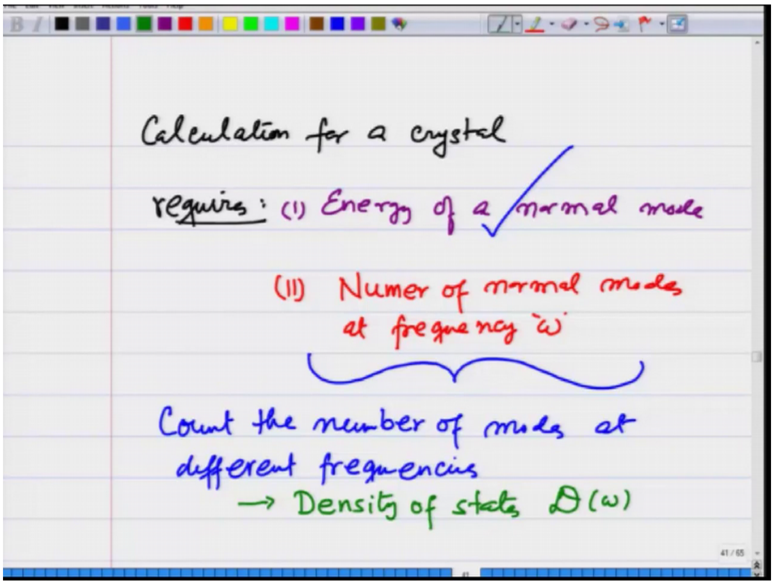

Calculation for a crystal

require : (I) Energy of a normal mode ✓

(II) Numer of normal modes at frequency 'ω'

$\underbrace{\hspace{6em}}$

Count the number of modes at different frequencies

→ Density of states $D(\omega)$

Now, if I want to calculate things for a crystal, so for calculation for a crystal, it requires number 1 energy of a normal mode and this is number 1. And it also requires number of normal modes at frequency omega, so I require two things. The first part I have done.

So, it is the second part that I am going to focus on in this lecture that is what we are going to count, what we are going to do is count the number of modes at different frequencies. You have done this in the past in connection with free electrons, we are going to repeat pretty much the same thing, but this is going to be in the context of vibrations.

And when I count the number of modes at different frequencies, let me remind you what you did in terms of free electrons. We are going to introduce something called the density of states D omega, so that D omega time’s delta omega gives you the number of modes between frequency omega and omega plus delta omega.

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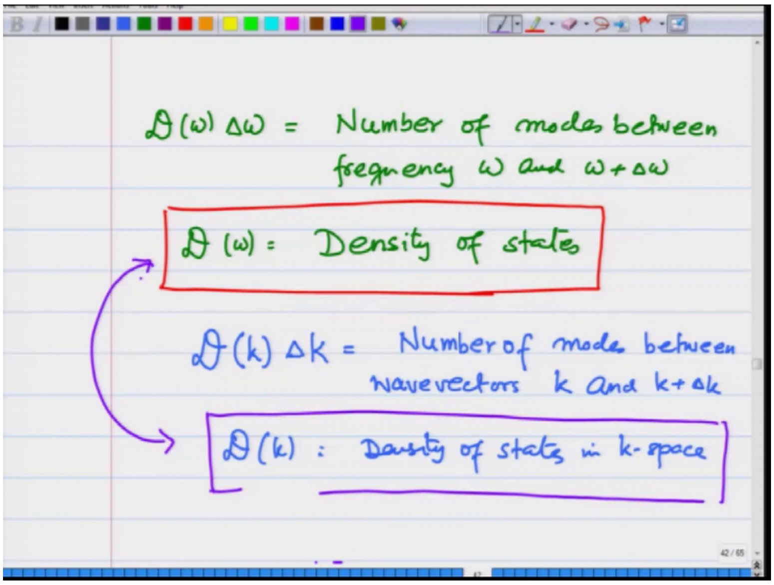

$\mathcal{D}(\omega)\,\Delta\omega$ = Number of modes between frequency ω and $\omega+\Delta\omega$

$\mathcal{D}(\omega)$: Density of states

$\mathcal{D}(k)\,\Delta k$ = Number of mode between wavevectors k and $k+\Delta k$

$\mathcal{D}(k)$: Density of states in k-space

So, let me now write this delta D omega delta omega gives the number of modes, these normal modes between frequency omega and omega plus delta omega. And D omega therefore is known as the density of states. These are not new definitions, you have encountered those in connection with free electron theory that Professor Banerjee did in the first part of the course. I am just going to reiterate the whole thing in the context of phonons.

At the same time when I want to do D omega, a concept that will be more useful. And we will lead to D omega; let me call it D k, so that D k delta k gives me the number of modes or number of states between wave vectors k and k plus delta k. So, D k I am going to call density of states in k-space, I do not want to use too many notations, so I am just calling with D k and D omega. And these two are going to be related, let us see how?

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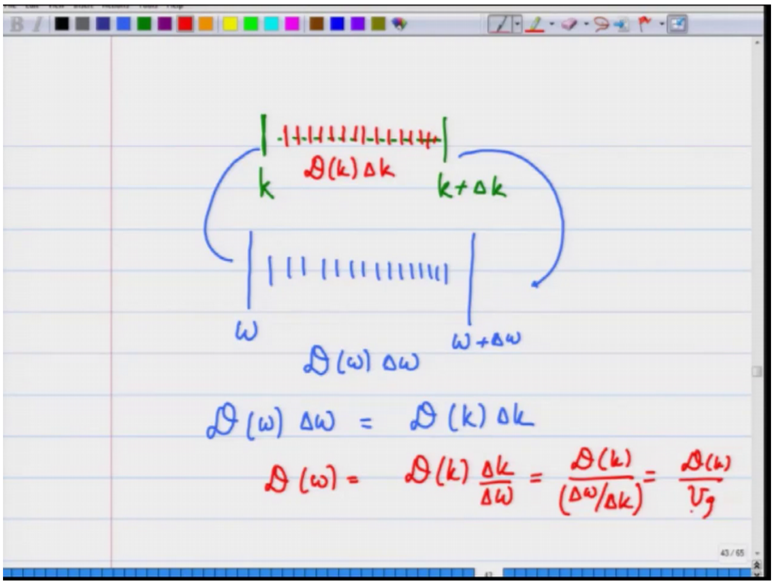

$$\mathcal{D}(\omega)\,\Delta\omega = \mathcal{D}(k)\,\Delta k$$

$$\mathcal{D}(\omega) = \mathcal{D}(k)\frac{\Delta k}{\Delta\omega} = \frac{\mathcal{D}(k)}{(\Delta\omega/\Delta k)} = \frac{\mathcal{D}(k)}{v_g}$$

If I have let say one k and slightly away from it k plus delta k and there are these states in between some number. Corresponding to k, there is an omega; corresponding to k plus delta k, there is a omega plus delta omega. These are corresponding to this k and k plus delta k and all these states are in between, so that the omega times delta omega and D k times delta k gives you the same number of states.

And therefore, what I have is density of states in omega delta omega is equal to density of states in k delta k or the omega is equal to D k delta k over delta omega, which is equal to D k divided by delta omega over delta k, recall that delta omega by delta k is the group velocity, so this D k divided by v group.

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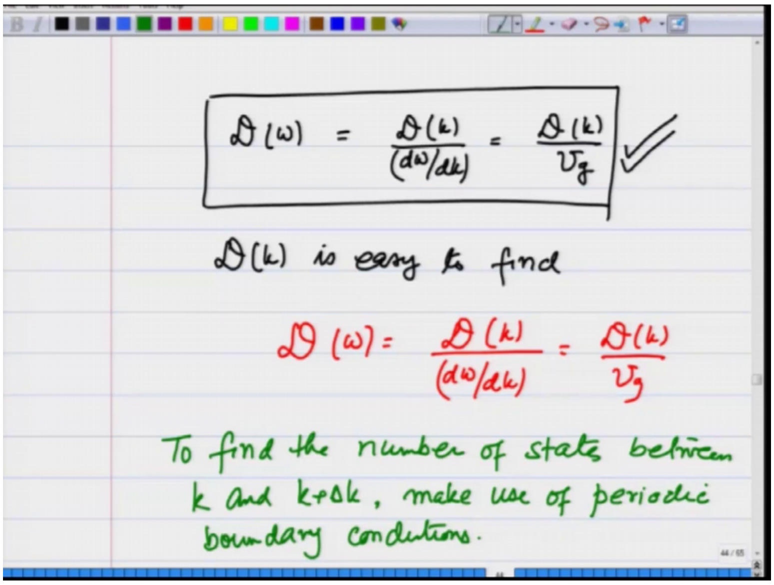

$$\boxed{D(\omega) = \frac{D(k)}{(d\omega/dk)} = \frac{D(k)}{v_g}} \checkmark$$

$D(k)$ is easy to find

$$D(\omega) = \frac{D(k)}{(d\omega/dk)} = \frac{D(k)}{v_g}$$

To find the number of state between k and $k+\Delta k$, make use of periodic boundary conditions.

So, what we found is that density of states D omega is equal to D k divided by d omega d k, I am just replacing the delta by the differential which is equal to D k over v group, this is how I find the density of states. Now, D k is easy to find, so we worked in terms of D k and then using the formula given here we obtained D omega. So, once I find D k, I get D omega, which is equal to D k over d omega d k, which is D k over v g.

So, all now I need to do is find D k, find the number of state between k and k plus delta k. And to do this to find the number of states between k and k plus delta k, we need to count them and what we use make use of as make use of periodic boundary conditions. Again the same tricks that you used in terms of electrons, now we are going to use the same tricks here in terms of phonons.

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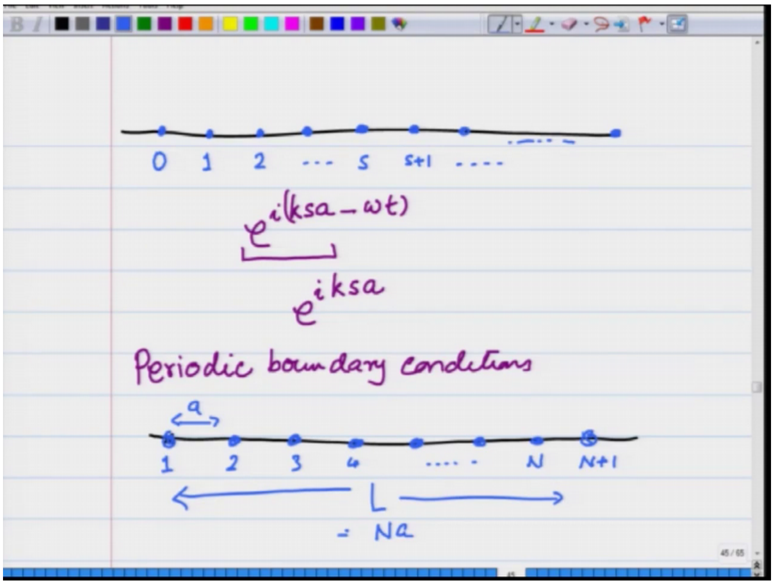

What are periodic boundary conditions? So, let us take in one dimension a long chain of atoms shown by blue here and so on. So, I have 0th atom, the first atom, the second atom, the sth atom, s plus 1th atom and so on. The wave or the displacement is given by e raised to i k s a minus omega t. I am right now going to ignore e raised to minus omega t part, because it is not important for periodic boundary conditions and focus only on this displacement at a given time.

So, displacement is given by e raised to i k s a. And in applying periodic boundary conditions, so to apply periodic boundary conditions, I look at this chain and consider n atoms, so again I am going to show them by blue 1, 2, 3, 4 all the way up to N and N plus 1th atom. If this distance is a, the length of the chain is L is equal to N times a, because they are going to be N gaps between first and N plus 1th atom.

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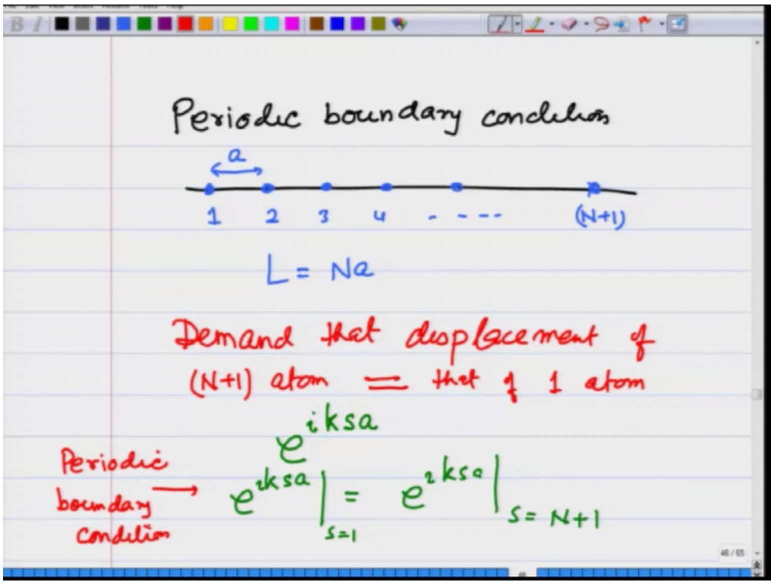

Periodic boundary condition

$L = Na$

Demand that displacement of (N+1) atom = that of 1 atom

e^{iksa}

Periodic boundary condition → $e^{iksa}\Big|_{s=1} = e^{iksa}\Big|_{s=N+1}$

And then what we do is so what we are discussing is periodic boundary condition for which I have considered this atoms 1, 2, 3, 4, all the way up to N plus 1th atom, so that the length is Na, a being the distance between neighboring atoms.

And to apply periodic boundary conditions, we demand that displacement of N plus 1th atom, the same as that of first atom. If that is the case, then what I am going to have remember displacement is given by I e raised to i k s a. So, what I am asking for is e raised to i k s a be equal to for s equals 1 be equal to e raised to i k s a for s equals N plus 1. This is the condition that I am demanding for periodic boundary condition.

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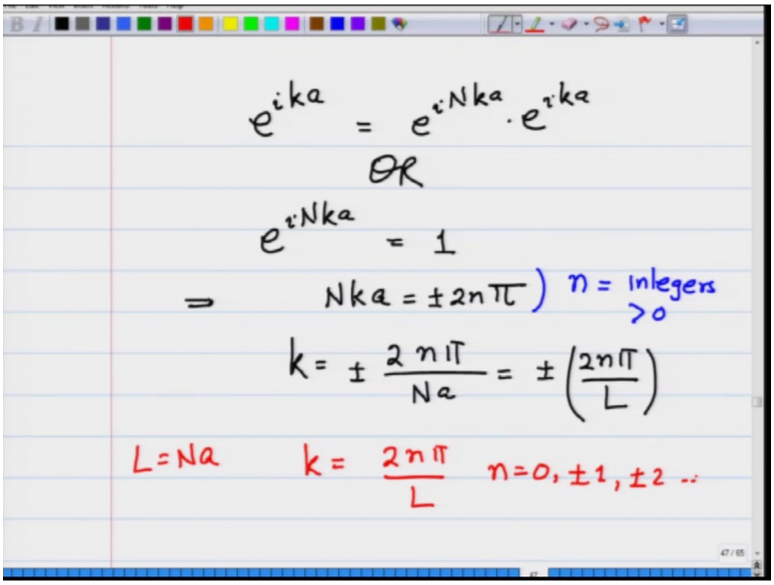

$$e^{ika} = e^{iNka} \cdot e^{ika}$$

OR

$$e^{iNka} = 1$$

$$\Rightarrow \quad Nka = \pm 2n\pi \Big) \quad n = \text{integers} > 0$$

$$k = \pm \frac{2n\pi}{Na} = \pm\left(\frac{2n\pi}{L}\right)$$

$L = Na \qquad k = \frac{2n\pi}{L} \qquad n = 0, \pm 1, \pm 2 \ldots$

So, what it gives me, I am asking for e raised to i k a for s equals 1 is e raised to i k a be equal to e raised to i N k a times e raised to i k a or e raised to i N k a be equal to 1. And this gives me N k a equals 2 n pi plus or minus. And therefore, k is equal to 2 n pi over N a plus or minus, which is equal to plus or minus 2 n pi over the length over which N atoms are there. Because, recall we had L equals Na and in this n are integers greater than 0 or 0. I could also have written this as k equals 2 n pi over L with n being equal to 0 plus minus 1, plus minus 2 and so on.

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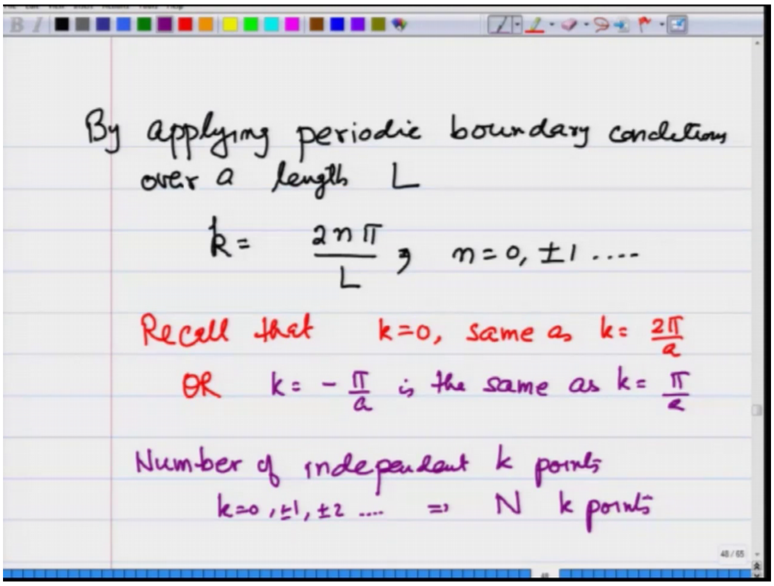

By applying periodic boundary conditions over a length L

$$k = \frac{2n\pi}{L}, \quad n = 0, \pm 1 \ldots$$

Recall that $k = 0$, same as $k = \frac{2\pi}{a}$

OR $k = -\frac{\pi}{a}$ is the same as $k = \frac{\pi}{a}$

Number of independent k points

$k = 0, \pm 1, \pm 2 \ldots \Rightarrow N$ k points

So, what we have found by applying periodic boundary conditions over a length L is that k equals 2 n pi over L with n equals 0, plus minus 1 and so on. Now, recall that k equal to 0 is same as k equals 2 pi by a or equivalently when we define the Brillouin zone is the same thing k equals minus pi by a is the same as k equals pi by a.

And therefore, we have number of case independent k points is k equal to 0, 1 plus minus 1, plus minus 2 and so on right. So, this gives me N k points. You going to say, it is n minus 1, it is not n minus 1, because 0 is also included. So, there are N independent k points and what are their values.

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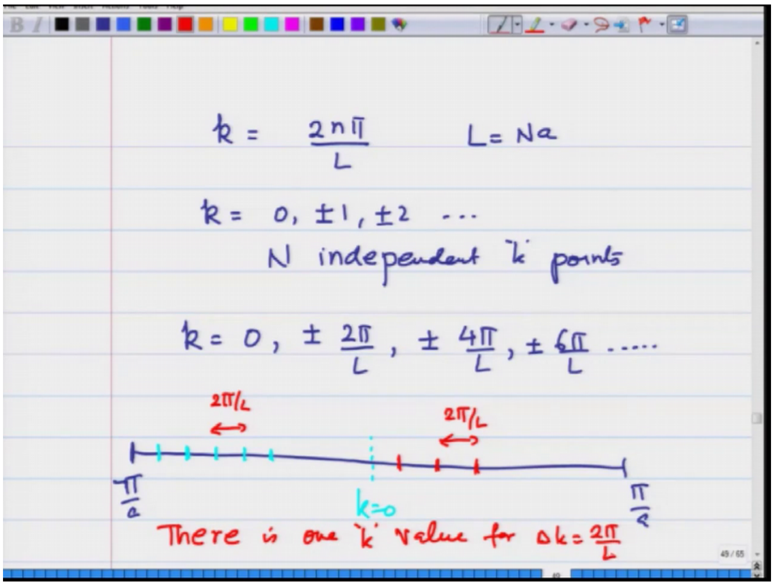

$k = \frac{2n\pi}{L}$ $L = Na$

$k = 0, \pm 1, \pm 2 \ldots$

N independent 'k' points

$k = 0, \pm \frac{2\pi}{L}, \pm \frac{4\pi}{L}, \pm \frac{6\pi}{L} \ldots\ldots$

There is one 'k' value for $\Delta k = \frac{2\pi}{L}$

So, k equals 2 n pi over L, L equals Na. And k equals, therefore 0, plus minus 1, plus minus 2, and so on. N independent k points and the values are k equals 0 comma plus minus 2 pi by L comma plus minus 4 pi by L comma plus minus 6 pi by L and so on. So, if I were to draw a line from minus pi by a to pi by a in the k-space, so if I were to draw this line in the k-space, there is 1 k value, let us say this is k equals 0, then 1 k value every 2 pi by L, this distance is 2 pi by L, this distance is 2 pi by L. So, there is 1 k value for delta k equals 2 pi by L.

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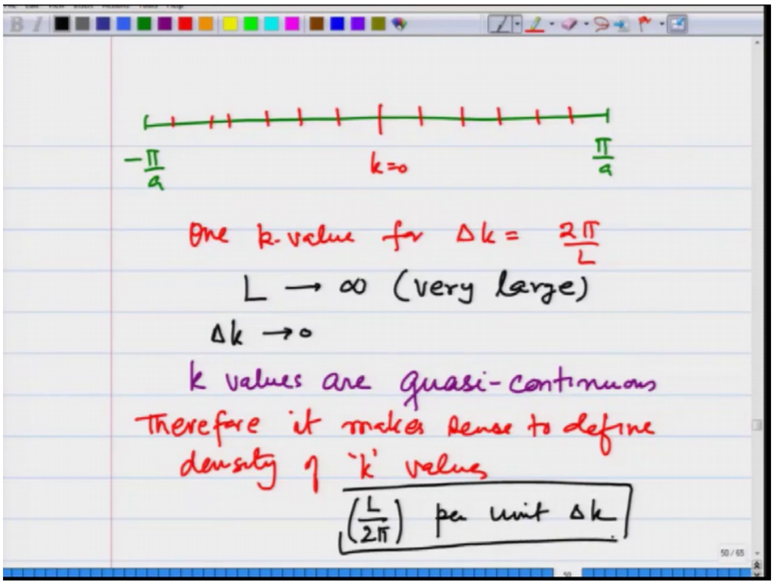

$-\frac{\pi}{a}$ $k=0$ $\frac{\pi}{a}$

One k-value for $\Delta k = \frac{2\pi}{L}$

$L \to \infty$ (very large)

$\Delta k \to 0$

k values are quasi-continuous

Therefore it makes sense to define density of 'k' values

$\boxed{\left(\frac{L}{2\pi}\right) \text{ per unit } \Delta k}$

So, in this line between minus pi by a to pi by a, this is k equal to 0. Every 2 pi by L there is one k value, for delta k equals 2 pi by L. Now, in applying boundary conditions periodic boundary conditions, we always keep in mind that L is tending to infinity is very large. So, delta k is almost going to 0, so these k values are quasi-continuous.

So, they are not like huge distances away from each other, they almost very close to each other, because L is tending to very large value and delta k is almost 0, so they are quasi-continuous. And therefore, it makes sense to define density of k values. So, I argued, why I can define density of k values and what will it be its very simply. There is one k value for every L by 2 pi, so it will be L over 2 pi per unit delta k.

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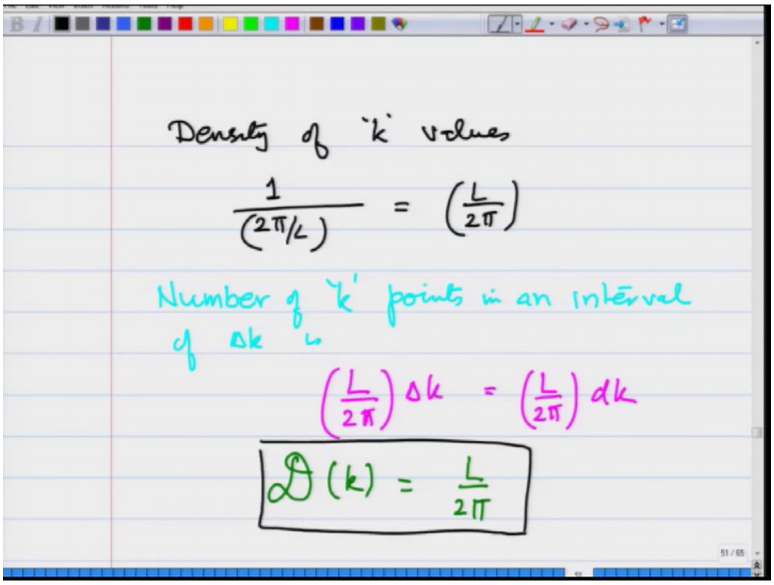

Density of 'k' values

$$\frac{1}{(2\pi/L)} = \left(\frac{L}{2\pi}\right)$$

Number of 'k' points in an interval of Δk is

$$\left(\frac{L}{2\pi}\right)\Delta k = \left(\frac{L}{2\pi}\right)dk$$

$$\boxed{\mathcal{D}(k) = \frac{L}{2\pi}}$$

So, let us write it again. So, density of k values is going to be 1 k value every 2 pi over L delta k, this is equal to L over 2 pi. So, I can now say that number of k points in an interval of delta k is going to be equal to L over 2 pi delta k or in the limit of delta k going to 0, this is equal to L over 2 pi d k. And this immediately tells you that D k is equal to L over 2 pi. So, this is the first result that we have gotten. Having obtained this, the next job is going to be to get D omega from this.