Introduction to Solid State Physics

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Lecture - 51

Calculating density of states of phonons; the Einstein's and the Debey models

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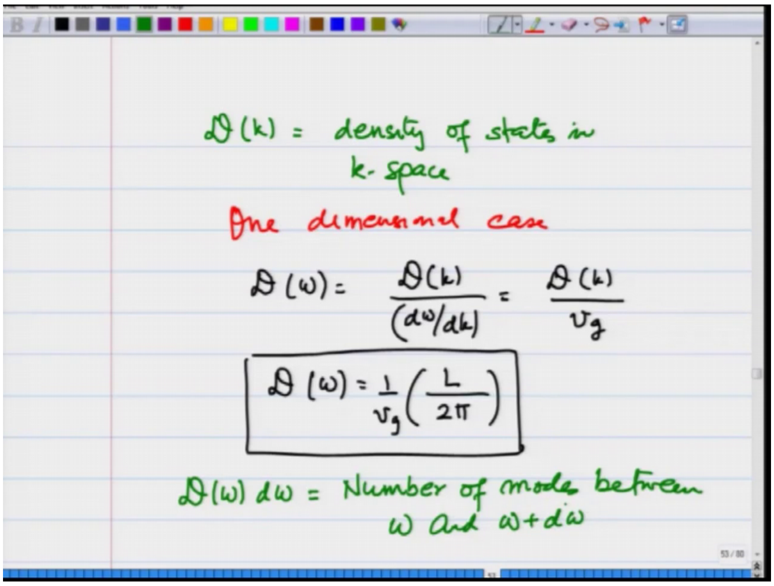

In the previous lecture, we obtained D k, which gives the density of states in k space. And we did it for one-dimensional case. We were also shown there that D omega is nothing but D k divided by d omega d k which is equal to D k over v g. So, having obtained D k, I can write D omega is equal to L over 2 pi 1 over v group that is my density of states in omega space, so that D omega times d omega gives number of modes between frequency omega and omega plus d omega.

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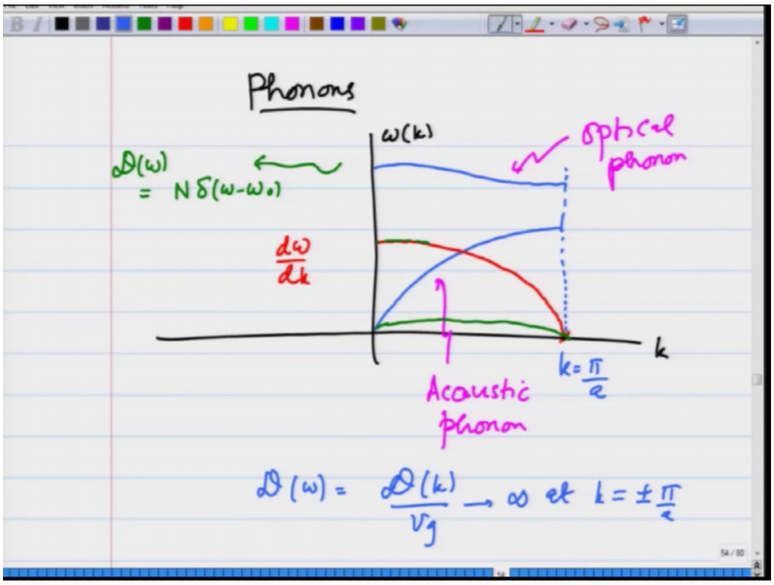

Now, recall that when we discussed phonons, this is all in the context of phonons, we had omega k versus k as acoustic phonons here, I am making only on one side the other side is symmetric this is k over k equals pi over a. And the other phonon like this, we call this the acoustic phonon, and this one optical phonon. And what you can see let us focus on acoustic phonon that d omega d k if I were to plot for acoustic phonon, and I will plot it right here if I were to plot d omega d k, you will see this is has a finite value and slowly becomes smaller and goes to 0 at pi over a.

In the case of omega k for the optical phonons also you can see that for the optical phonons it will be almost 0 here and d omega d k 0 goes to very small value and goes to 0 again. In fact, to a good approximation here I can write D omega as N delta omega minus omega 0, I will explain that in a minute.

Here there is some finite value and then vg goes to 0 here. Now, you see if I were to calculate the omega from D k divided by v g, it goes to infinity at k equals plus minus pi by a, it blows up. I need a model through, which I can work and which is a reasonable model and this is what we are going to do in this lecture.

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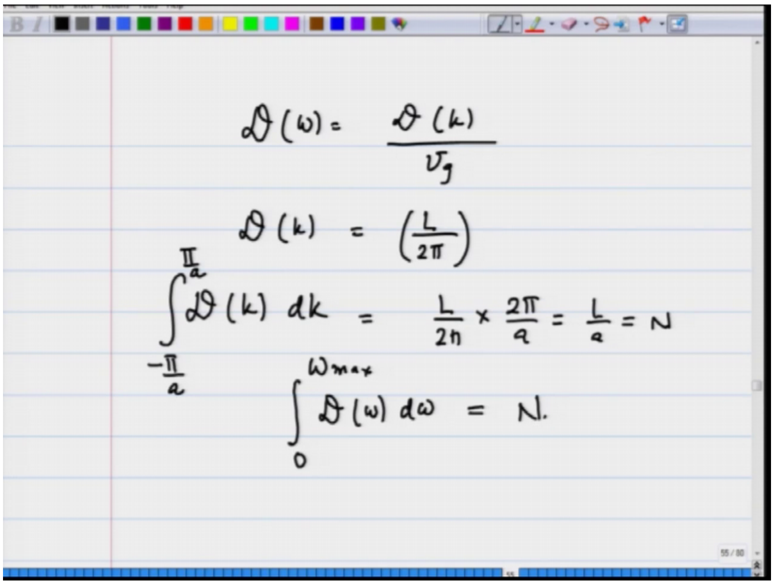

So, we had derived the omega, which is D k over v group D k is equal to L over 2 pi. If I integrate the density of states from k equals minus pi by a to pi by a, it must lead to the total number of modes which is does, because this is going to be L over 2 pi times 2 pi by a, which is L over a, which is equal to N. Similarly, if I integrate D omega from omega equals 0 to some omega max, it should give me N. So, we will be working through these equations, we have understood the meaning of the density of states, we have understood what it integrates to, and through these now we will be doing the calculations for energies and things like those.

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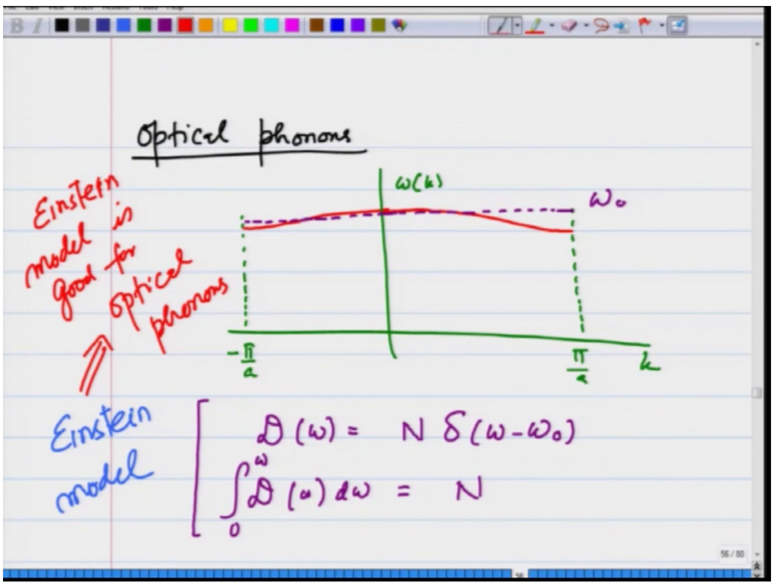

Now, as I said earlier if I were to look at the optical phonons, what we see is that omega k versus k if I were to plot it up to some point pi by a here, it is almost flat like this same thing on the other side almost flat. And you can see that there is only one omega I mean if I approximated this we can say one omega some omega 0 at which all the atoms are vibrating and therefore, I can just by inspection write D omega as number of modes delta omega minus omega 0.

So, that when I integrate D omega over this range 0 to some omega the point including omega 0 the number of modes come out to be precisely the same as the number of atoms in that chain of length l which it should be. So, this is a very simple model of density of states and this is known as the Einstein model. There is another model for the density of states which, I will call Debey model which I will explain next, but first the Einstein model this is good right I can see it right away. So, Einstein model let me write it on the left side of the screen, Einstein model it is good for optical phonons, because in optical phonons the, the frequency is almost constant.

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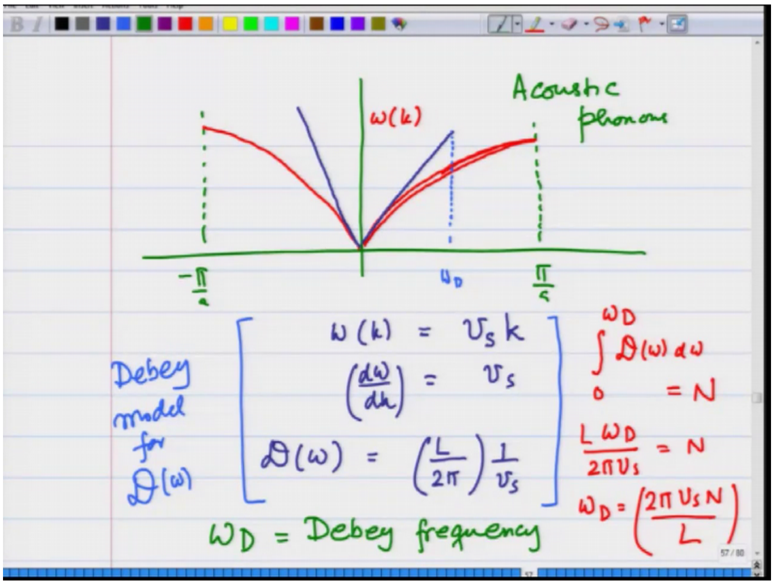

The other photons that we had was acoustic phonons. And here what we had was if I go up to pi by a, and here is minus pi by a, the omega versus k graph looks like this. In this case doing a calculation with all the dispersion here v g changing continuously becomes difficult. So, an approximation is made whereby I take the dispersion to be linear like this. In this case what we do is we take omega k is equal to the speed of sound times k, so that d omega d k becomes v s. And density of states in one dimension becomes L over 2 pi 1 over v s that is it this is known as Debey model, obviously it is an approximation.

And there has to be a maximum omega D or Debey there has to be a maximum omega max, so that integration 0 to omega D this is omega max D omega, D omega is equal to N. Therefore, you get L omega D over 2 pi v s equals N and omega D is equal to 2 pi v s N divided by L. So, when I make this approximation, the Debey model for D omega there is a maximum omega D up to which the modes go, because after that all the atoms all the number of modes, which are N is exhausted. So, there is a maximum frequency omega D, which is known as the Debey frequency. So, we have introduced a new term called omega D, which is Debey frequency.

So, I have given you the idea of two models of calculating D omega from d k Einstein model and D by model in one dimension, real crystals are three-dimensional. So, now, we will work these things out for three-dimensional crystals.

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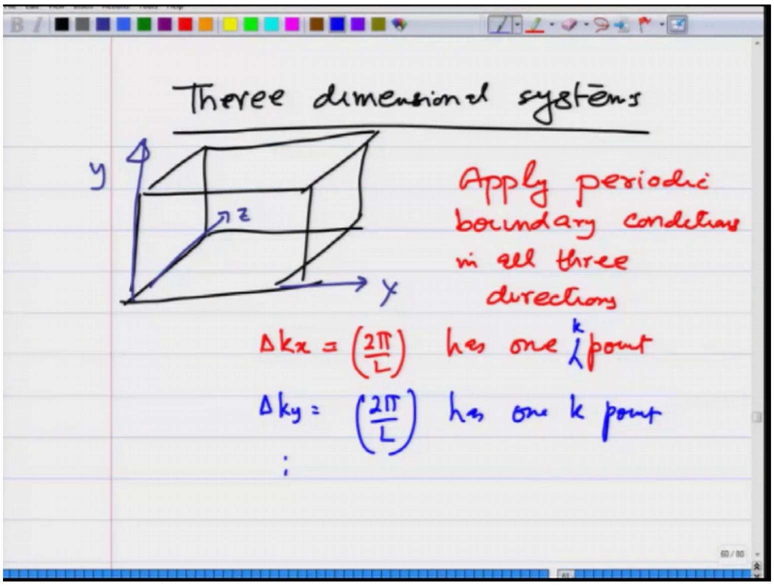

So, let us now consider the case of three-dimensional systems, where the crystal extents all three-dimensions in the x-direction, in the y-direction and in the z-direction. And then we apply periodic boundary condition in all three directions, what would this give me, this will give me that delta k x with 2 pi over L has one point, one k point delta k y equals 2 pi over L has one k point and same thing for delta k z.

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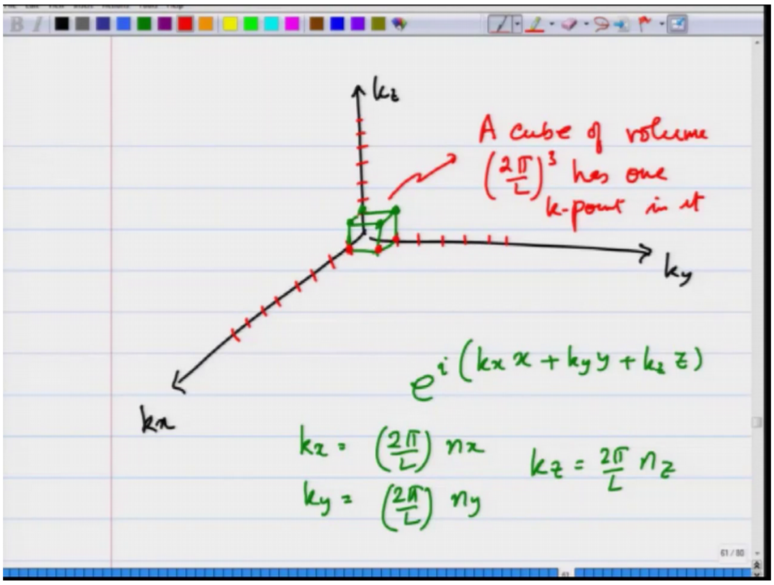

Let me show it pictorially. So, if I have this k x, k y, k z there is one every 2 pi by L there is one k x point, every 2 pi by L there is one k y point, every 2 pi by L there is a k z point. How so because my way the displacement is e raised to i k x x plus k y y plus k z z minus omega t, which I am ignoring right now. So, in general, then there will be one point also at all these corners of the cube, because k x is equal to 2 pi by L times n x, k y is 2 pi by L n y, and k z is 2 pi by L n z. So, every time every n x, n y, n z integer gives me one point.

What we can say from this that I will write it here in orange a cube of volume 2 pi by L cube has one k point in it right. Either I can think of it that each k point has one-eighth coming into the cube or I can surround one point by this cube around it. So, a cube of volume 2 pi by L cube has one k point in it.

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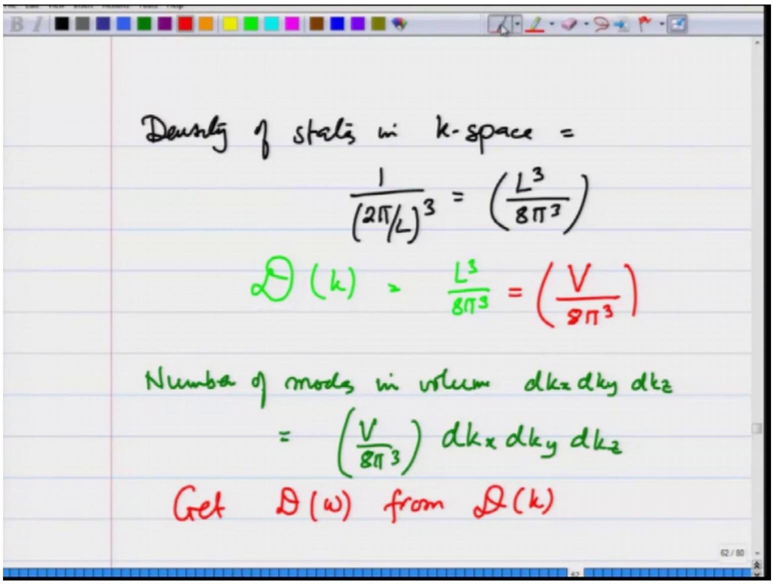

And therefore, the density of states in k space is going to be 1 over 2 pi by L cube, which is L cubed over 8 pi cube. So, we found D k to be L cubed over 8 pi cube, which is also written as L cube is the volume of the crystal over 8 pi cubed. And number of modes in volume d k x, d k y, d k z is equal to v over 8 pi cubed times d k x, d k y, d k z. And my next job is to get D omega from D k. How do we do that, I will take a very simple calculation.

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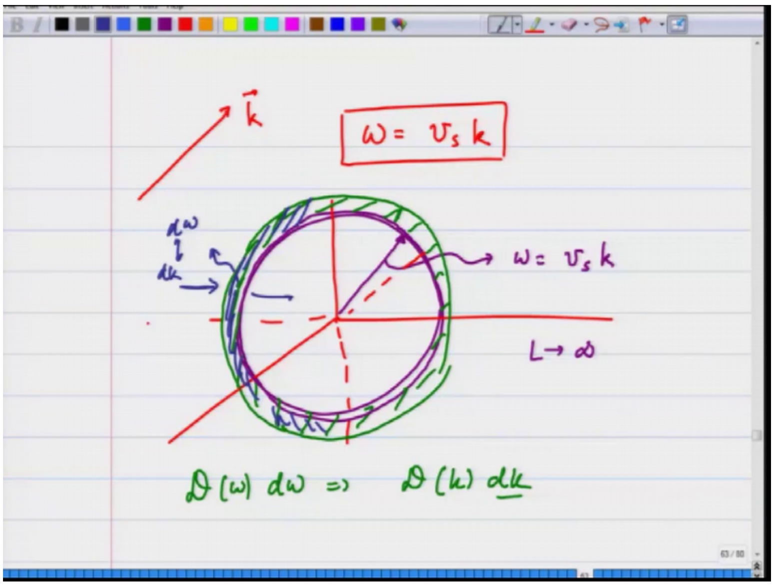

Now, recall that if there is a phonon propagating in direction k, I am going to have omega equals v sound k. I am taking things to be isotropic. And if I now look at this k space add some large value of k right, omega is going to be given as v s k. Recall from your lecture on 1 d that L is really going to infinity. So, these cubes are very, very small. So, if I were to look at one particular omega, I can take this line which gives me one particular omega to be almost spherical in fact perfectly spherical in the limit of L going to 0. What I want to count is, what is the number of modes between omega and D omega, I want to count the number of modes in this shell.

And that is quite easy number of modes in this shell is going to be equal to D k times d k, where d k corresponds to this width out here, this width out here in the radius in the k space d omega corresponds to d k. So, what I need to do is actually count the number of modes in this volume of k space, where the radius of this the shell is d k in k space, and that will give me D omega in omega space.

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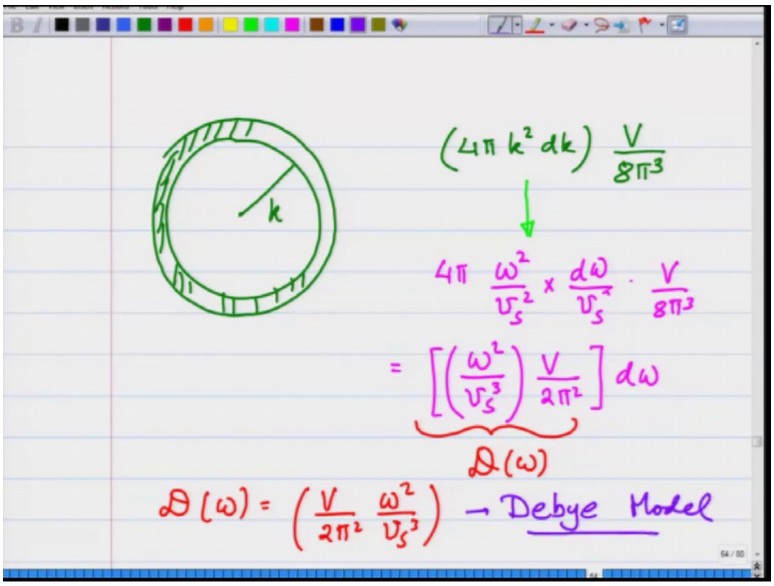

So, if I look at this sphere of radius omega a correspondingly k in the k space and count the number of modes in this volume, this volume is 4 pi k square d k, and the number of modes in this is going to be v over 8 pi cubed. Now, let us translate this into omega space, and this comes out to be 4 pi k is nothing but omega square over v sound square times d k is nothing but d omega over d v sound times v over 8 pi cubed, which I can write as omega square over v s cubed times v over 2 pi square d omega.

And this is nothing but by definition D omega. So, D omega is equal to v over 2 pi square omega square over v s cubed. And remember in this case we assume that omega equals v s k. So, this is the Debey model.

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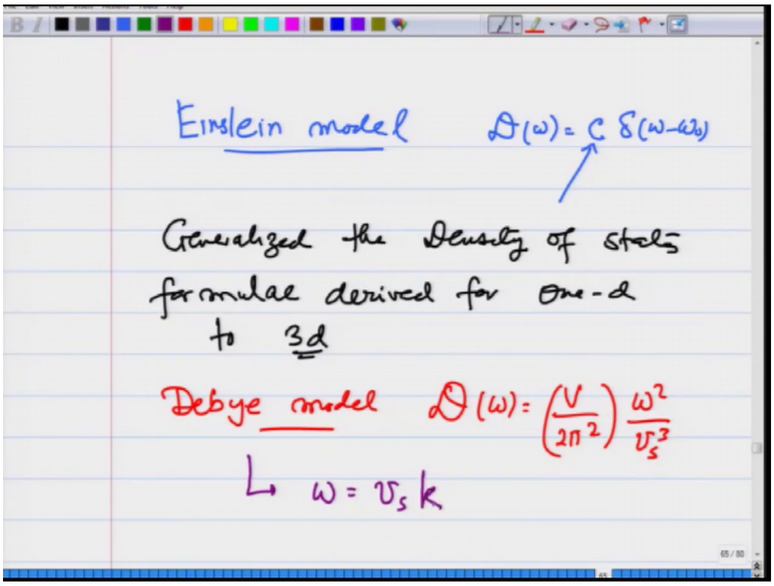

The Einstein model in which case omega is almost a constant remains the same, this equals you know whatever some constant times delta omega minus omega 0, I am writing this constant, because in 3D the number of modes would be different. So, what we have done in this lecture is generalized the density of states formulae derived for 1D to 3D. And in particular the Debey model, we got D omega equals v over 2 pi square omega square over v sound cube. Now, what is Debey model? In this we assume that omega is v s times k.

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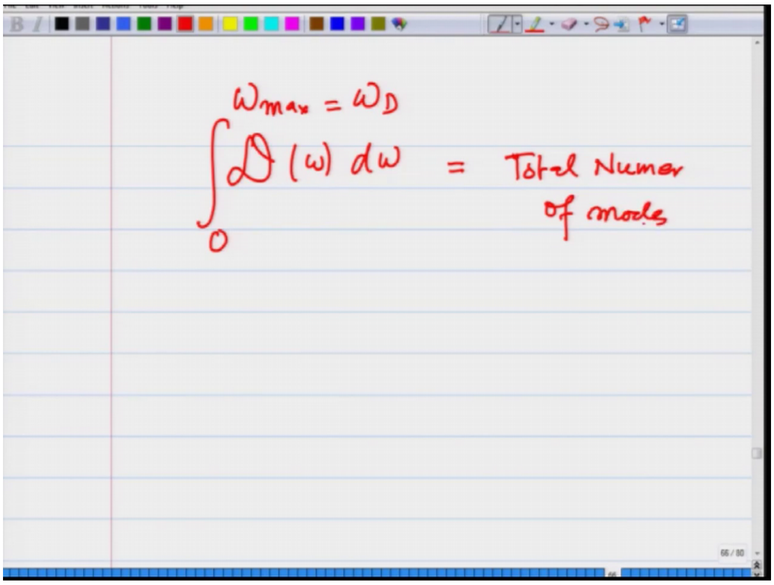

Now, obviously when I have this D omega, it integrated over from some omega equals 0 to omega max, which I am called going to call the omega Debey should integrates to the total number of modes.