Introduction to Solid State Physics
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Lecture – 46
Normal modes in a crystal : Phonons and their momenta and energy

Having covered all the preliminaries of crystal vibrations in the lecture so far, what I want to do now is introduce more concepts.

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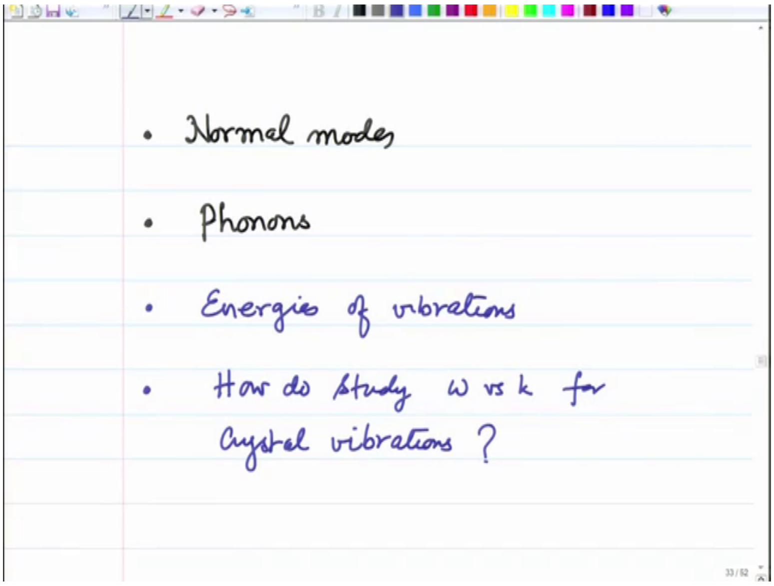

And the concepts I want to introduce are those of Normal modes and Phonons and also now start worrying about energies of vibrations. And how do we study omega versus k for crystal vibrations? Why are these things important, because these actually define I have already introduced the idea of speed of sound being the slope of omega versus k near 0 k equals 0 for a crystal. So, they also define other properties, I can relate speed of sound to the bulk modulus and so, on they give us information about the force between the atoms or planes in a crystal.

So, these things become important. So, let me develop them slowly in this lecture in the next. You notice that when these atoms are vibrating so, let me make these atoms, it is not an individual atom that is vibrating they actually the whole lattice all atoms are vibrating together in a pattern.

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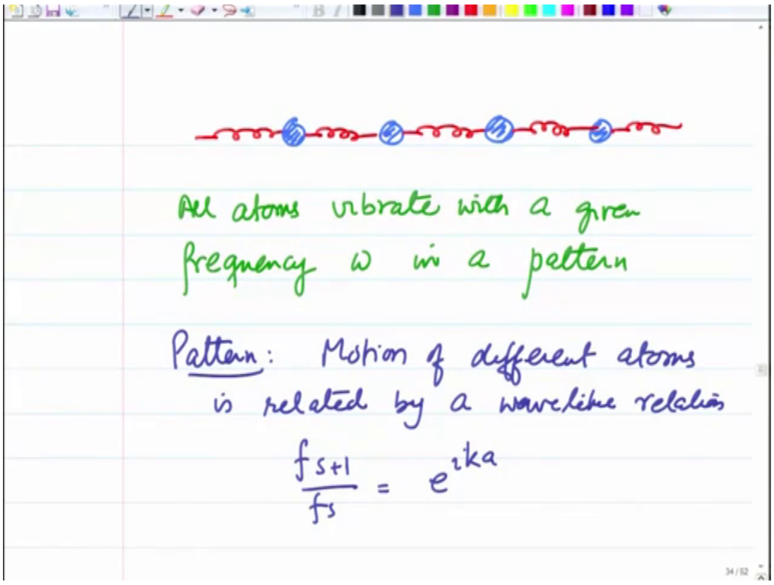

So, all atoms vibrate with a given frequency omega in a pattern. And what is the pattern? Pattern is that the pattern is that the motion of different atoms is related by a wave like relation that is f s plus 1 over fs is going to be equal to e raised to i ka or the real part of it. So, they are all related; so, this whole thing is vibrating with one frequency something like what you are already familiar with.

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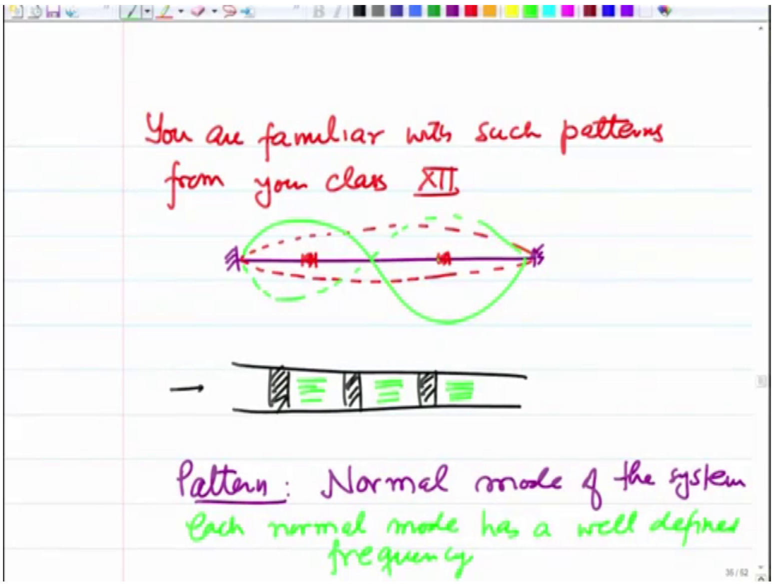

So, let me show you what you are familiar with. You are familiar with such patterns from your class 12. And what is that? Consider a string between two ends and vibrating, right.

When it vibrates, it can vibrate in his fundamental mode like this, it can vibrate in the next harmonic like this, right. In this case the individual parts of this string are related by this phase relationship as if there is a wave traveling, right.

So, what you have studied in the past is that I can consider this as standing wave which is a superposition of two traveling waves. So, each part of this string for example, this part and this part, their motion is related by a wave like relationship. So, this is a pattern and this pattern is known as normal mode. Another example is when you take an organ pipe. In an organ pipe when you blow or make sound there are high pressure zones low pressure zones and so on.

So, let me show by black the high pressure zones and by this green the low pressure zones and they also occur in a wave like pattern. So, its not individual particle like vibration, but the whole thing is vibrating and it is vibrating in a pattern and this pattern is called normal mode of the system. And each normal mode has a well defined frequency. So, whenever I take an extended system like the string out here or an organ pipe or my crystal planes they all participate in this, this vibration and this vibration has a well defined frequency omega.

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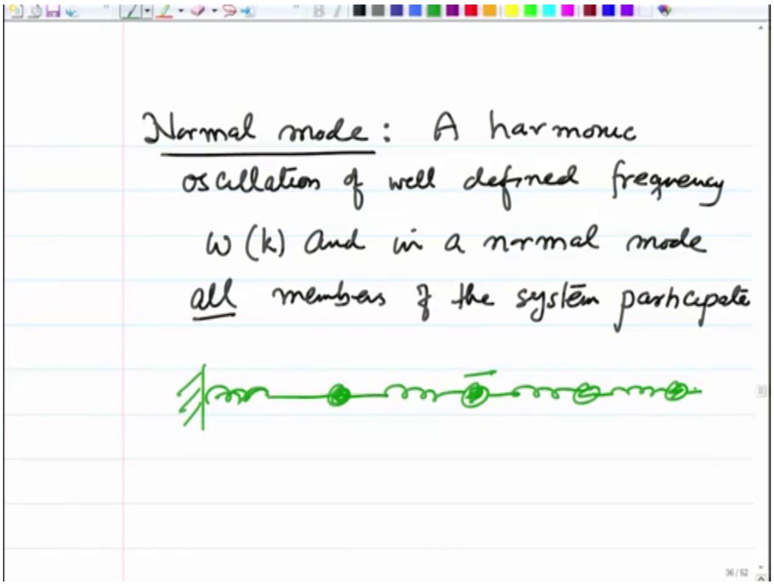

So, this normal mode is a harmonic oscillation of well defined frequency omega that we will depend on k, because this pattern has a k related with it, right. So, it is well defined frequency omega k and in a normal mode all members of the system participate. An example of a normal mode that we gave in your 0 th assignment was these two masses connected by a spring to a wall. So, it was not the frequency of one particle oscillating do both particles were participating and you got two frequencies, there were two normal modes. When you make this long you get many, many more normal modes and those are omega k right different frequency are given as omega k. And each normal mode is defined by a k. How many normal modes exist? You can actually guess from there it will be equal to the number of particles, but we will defer it for some time. So, we define a normal mode.

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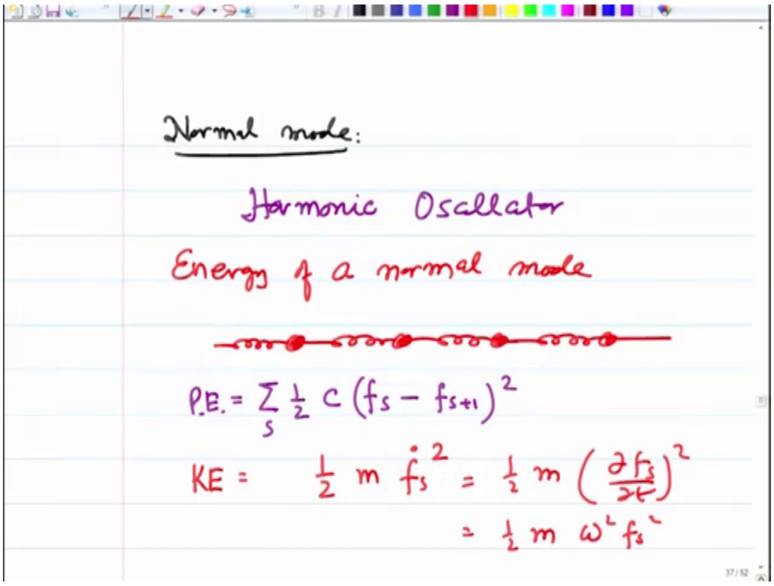

Now, let us see what we want to do next. We want to look at this normal mode which I have said is like a harmonic oscillator. And what about the energy of this normal mode of normal that is easy to calculate. If I have, I will go back to this model of this atoms in 1 d. If there is only nearest neighbor interaction then the potential energy of the sth atom would be f s minus f s plus 1 square, it does not matter whether I take f s plus 1 minus f s or f s minus f s plus 1, because I am squaring it one half C and I sum over s this will be the potential energy of the normal mode. If I have all the planes interacting, I will add other terms which I will give as an assignment problem.

So, that will be an assignment problem for the other all the planes interacting, but this is what it is this is the potential energy. How about the kinetic energy? Kinetic energy I know is one half m f s dot square which is one half m df s by dt square and this will be one half m omega square f s square. So, it is exactly like harmonic oscillator. So, energy is going to be like harmonic oscillator.

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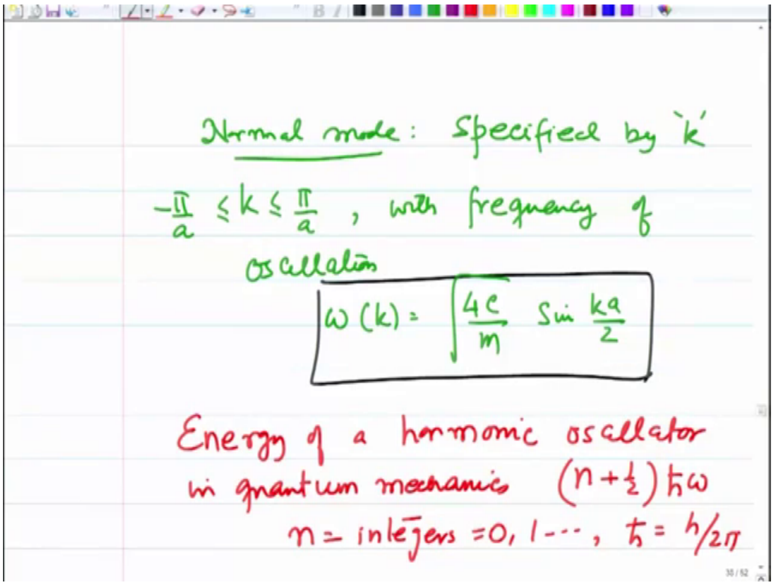

So, let us write again normal mode specified by k, right. And k is going to be pi over a minus pi over a restricted between these two limits with frequency of oscillation omega k being equal to in that nearest neighbor interaction limit 4 c over m square root of sin ka by 2.

Now, it so, happens that the energy is that a harmonic oscillator takes in quantum mechanics is n plus half h cross omega. So, energy of a harmonic oscillator in quantum mechanics is given as n plus a half h cross omega where n are integers 0, 1 and so on. H cross is h over 2 pi this is the energy of a harmonic oscillator. You can explain a lot of properties of crystals if you also take these normal modes to assume energy according to quantum mechanics.

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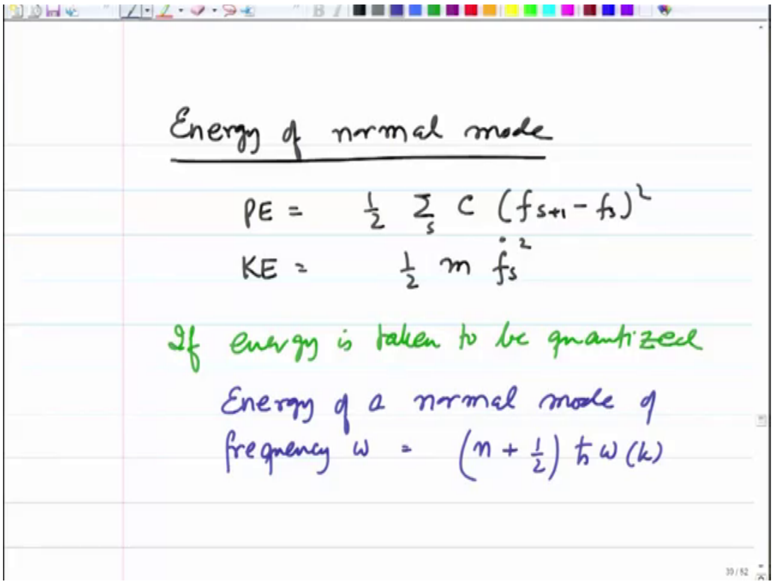

So, energy of normal mode, I wrote earlier that PE is equal to one half summation over s C fs plus 1 minus fs square and KE is one half m fs dot square, but it has explained long ago in the context of specific heat of solids by Einstein that you can explain specific heat only if you take if energy is taken to be quantized. So, we do not consider the classical expression, but rather we will write the energy of a normal mode of frequency omega to be equal to n plus a half h cross omega k.

So, these vibrations that are taking place in a crystal the energy of these vibrations cannot be just anything which is allowed by classical mechanics. It is given quantum mechanically that explains a lot of things. So, we take it for granted now that this is going to be the energy of the normal modes. And therefore, the energy of a normal mode is either h cross omega by 2 or 3 by 2 h cross omega or 5 by 2 h cross omega and so on, right which is all together n plus a half h cross omega.

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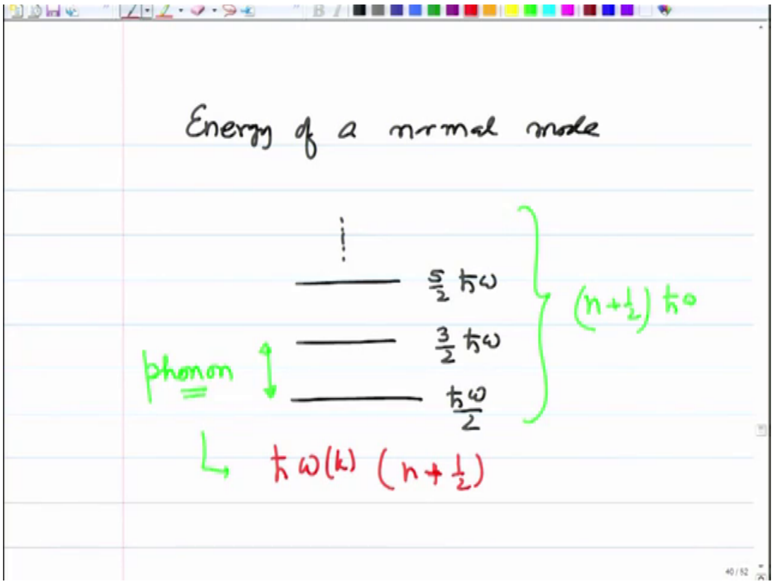

So, it can take energy in quanta of h cross omega and each of this quanta of energy is known as phonon. In correspondence with photon which is the quanta of energy of light, quanta of these vibrations or these waves that are traveling in a crystal is now going to be known as phonon. And each phonon just like a photon can take energy h cross omega k times n plus a half, no more no less this is what explains a lot of properties of crystals and therefore, we treat them quantum mechanically. So, this is the concept of phonon.

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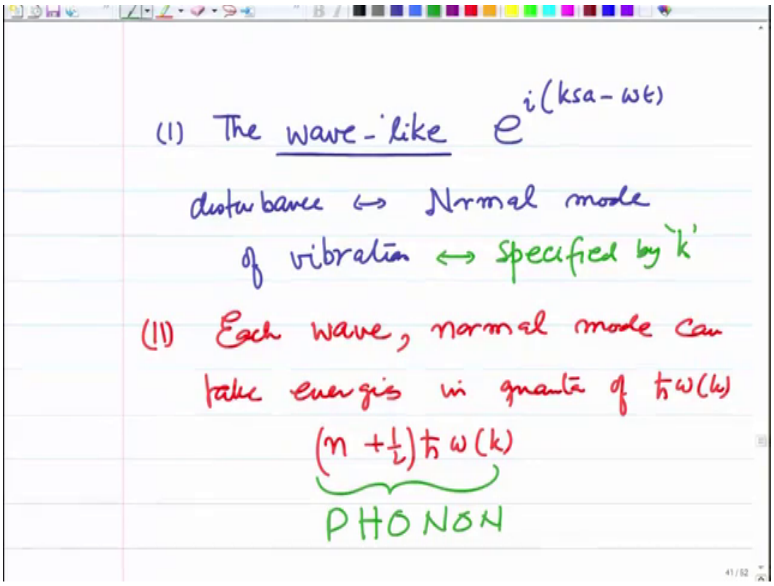

So, I introduced you to the idea of phonon. So, let us collect our thoughts together one the wave and I would say wave like, because it is actually not wave in the sense of continued media. So, the displacement is given by a k s a k s a minus omega t, this wave like, right a wave like disturbance it is normal mode of vibration.

And number 2 is this, each wave or normal mode can take energies in quanta of h cross omega k and energy is one half n plus a half h cross omega ok. And each normal mode is specified let me write it in green here on top of the screen again specified by k and k is restricted between minus pi by a and pi by a and this is known as phonon.

So, I can think, it does a quantum mechanics as if this crystal which is vibrating is filled with phonons like a cavity which is filled with light is filled with photons. So, I can think of this crystal as filled with phonons.

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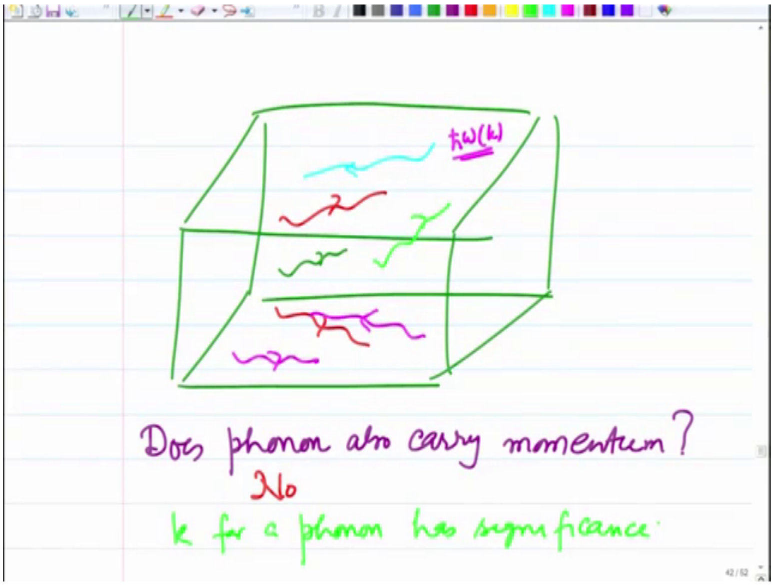

And if I have this crystal, it is filled with photons phonons going in all directions where the planes can vibrate. This is like these waves, it is filled with these phonons and each phonon carries energy h cross omega k, I this is excited and question is if it is a wave does phonon also carry momentum? Because you have learned in electromagnetic theory that a photon carries momentum also does phonon also carry momentum and the answer is no.

The simplest way of thinking about it is that suppose I have a wave where the particles are you know traveling in the its a transverse wave. So, particles are moving in direction perpendicular to the wave naturally it does not carry any momentum in the wave direction, because the motion is perpendicular to the wave direction.

So, phonons do not really carry any momentum. For longitudinal waves also you can show that if you sum over all the velocities and all the displacement over all the particles the sum will come out to be 0. So, it does not really carry any momentum; however, there is a difference k still for a phonon has significance of momentum.

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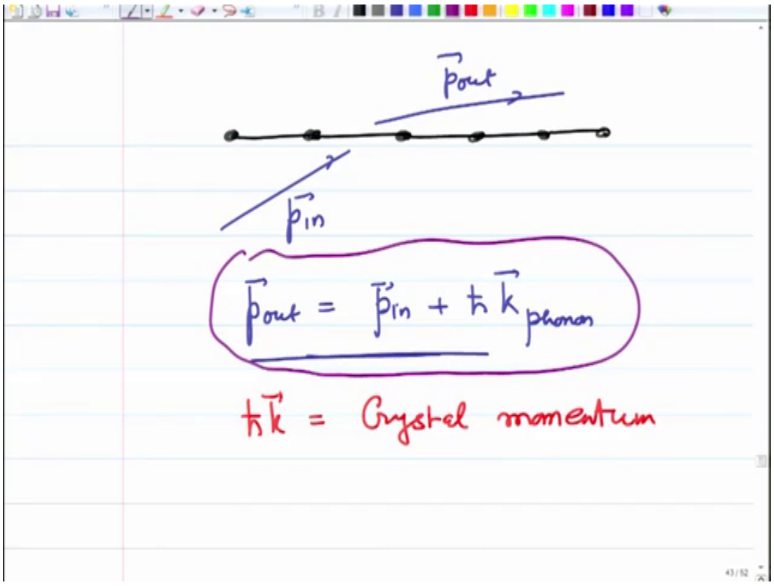

How so? If I have and I will again make this one dimensional lattice. If I have this lattice and I scatter some particle or way from it. And suppose incoming momentum was p in outgoing momentum was p out then it is seen that p out it is actually equal to p in, this is shown quantum mechanically. And later in the next lecture, I will also derive it in a very simple way by intuitive arguments is plus h cross k phonon.

So, this k of phonon behaves like it is representing the momentum. However, there is no momentum in phonon, it is just that it comes out when you really take the interaction of the incoming particle and the lattice into account. So, all the time this h cross k is given a name and it is known as crystal momentum that is in a crystal when particles interact the h cross k behaves like momentum. So, this law which is given here which I am encircling in purple can also be called the momentum conservation law. Having done that let us estimate what these numbers are going to be like.

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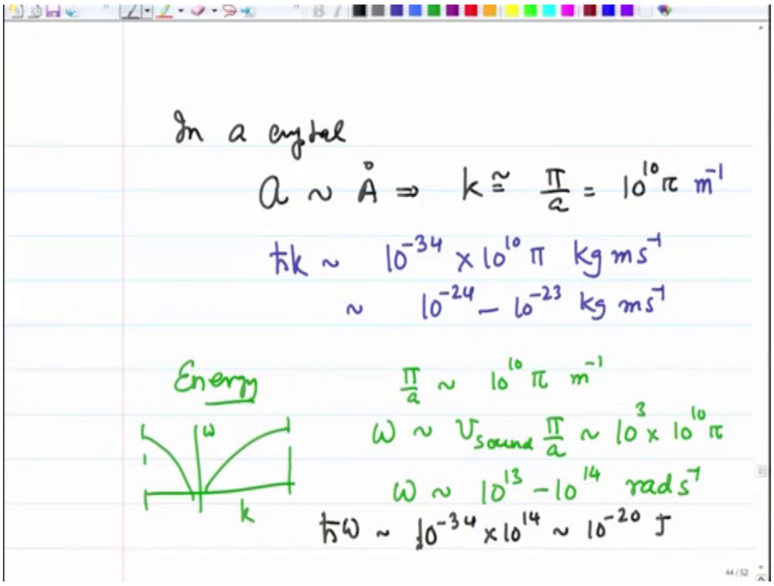

So, in a crystal, the particle distance is of the order of angstroms. And therefore, k is going to be of the order of pi over a which is 10 raised to 10 pi meter inverse and h cross k therefore, is going to be of the order of h cross is of the order of 10 raise to minus 34 times 10 raised to 10 pi kg meter second inverse which is 10 raise to minus 24 to 10 raise to minus 23 kg meter second inverse, that is the kind of momentum transfers we are looking for when the particles are scattered from this. How about the energy?

As I said earlier if you look at this graph of omega versus k pi by a is of the order of 10 raise to 10 pi meter inverse. And I can say that the frequency omega will be of the order of V sound times pi by a, right, because this is the relationship we had found near k equals 0. So, I may as well multiply by that and V sound is of the order of 10 raise to 3 meters per second in a solid times 10 raise to 10 pi.

So, omega is of the order of 10 raise to 13 to 10 raise to 14 radians per second. And therefore, h cross omega which is the energy of a photon is of the order of 10 raise to minus 34 times 10 raise to 13 to 14. So, let us try 10 raise to 14, 10 raise to minus 20 Joules.

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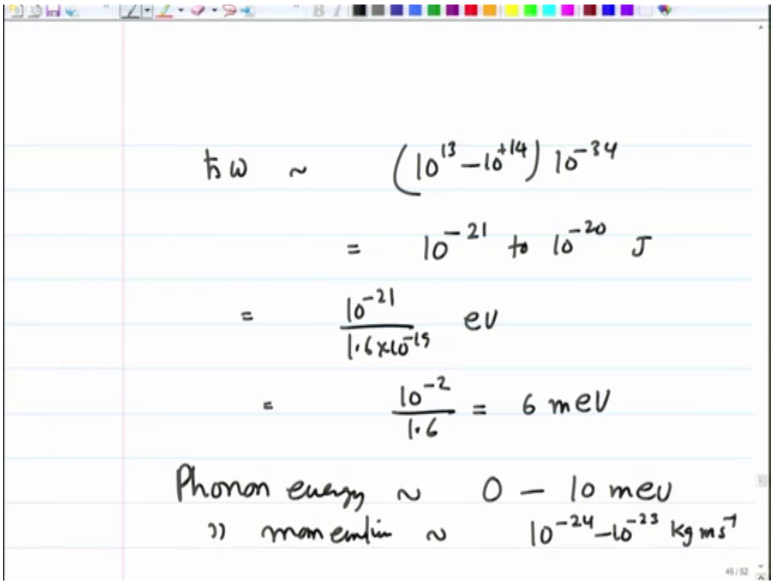

So, what we found is that h cross omega is of the order of 10 raise to 13 to 10 raise to 14 times 10 raise to minus 34 which is 10 raise to minus 21 to 10 raise to minus 20 Joules and that is then equal to roughly 10 raise to let us say minus 21 over 1.6 times 10 raise to minus 19 electron volts which is 10 raise to minus 2 over 1.6 and that is roughly 6 meV.

So, we can say that the phonon energy is of the order of 0 to 10 meV and phonon momentum is of the order of 10 raise to minus 24 to minus 10 raise to minus 23 kg meter second inverse, these are the kind of numbers for energies and moment we are talking about in a lattice. In the next lecture, we will see how we can determine the phonon spectrum omega versus k dispersion relationship experimentally.