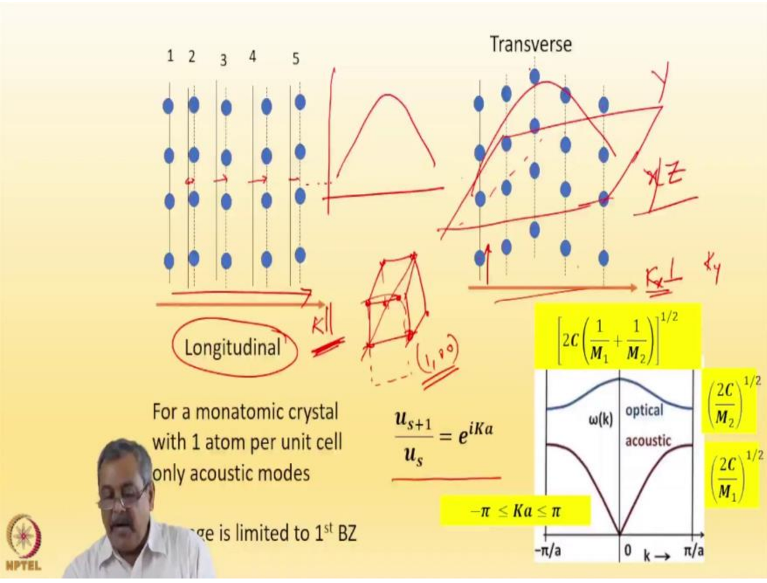
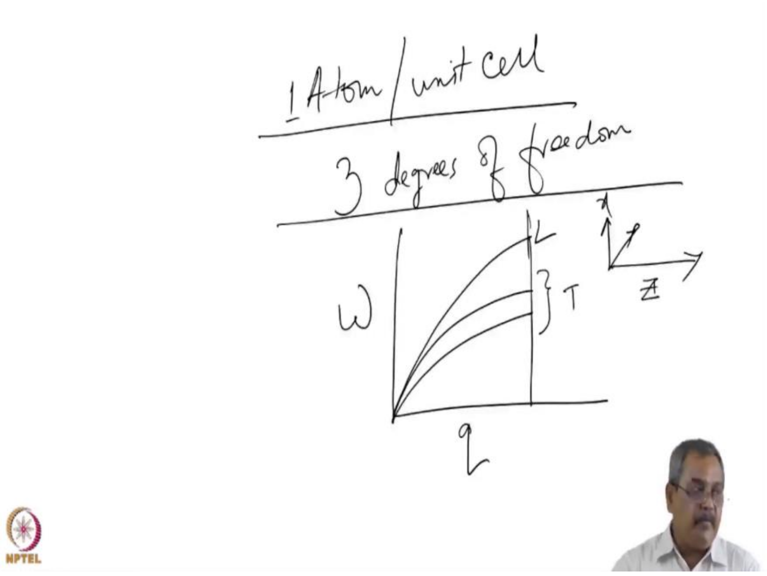
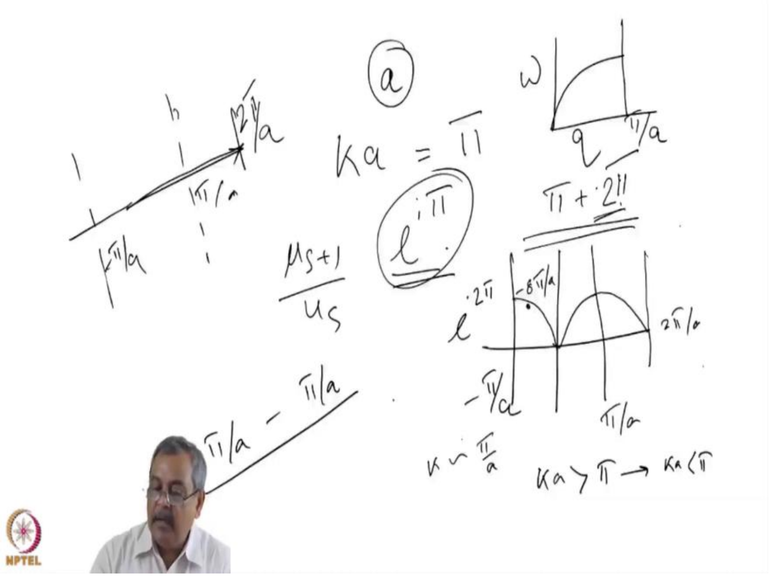
Neutron Scattering for Condensed Matter Studies
Professor Saibal Basu
Department of Physics
Homi Bhabha National Institute
Week 10: Lecture 25C

Keywords: Dispersion relation, Acoustic modes, Triple-axis spectrometer, Monoatomic crystal

(Refer Slide Time: 0:13)







If I take a plane of atoms, for example if it is a simple cubic lattice with atoms at the corner then I can talk about planes of atoms such as diagonal planes of atoms or (1 0 0) plane of atoms and so on. Hence, I can talk about various planes of atoms.

Here, displacements shown in left side of figure is one way of showing the longitudinal displacements. That means this is one plane I have shown as a line in the plane of the board, the next plane is displaced by some amount and the next to next plane is displaced little more and the next plane a little more so the wave is going to the highest amplitude then it starts reducing and so on. Here the displacement is along the propagation vector (of the phonon). Hence if propagation vector is K and the particle movement is parallel to K then it is known as longitudinal mode.

On the other hand, this displacement from one plane to another can also be in a direction normal to the propagation vector. Here I just take one example of the plane where the movement, say in the xz-plane. The atoms from this plane to this plane are displaced up, next plane is displaced further up then in the next plane it comes down and possibly in the next plane it comes to initial value. So, you can see a sinusoidal chain. But here the propagation vector is perpendicular to the direction of displacement, hence this is a normal displacement. Similarly, I can think of another plane, let me just draw it here which is perpendicular to the xz-plane, let me call it y direction and the same displacement of the atomic planes I can conceive in the y direction and the propagation direction in z so then also we have normal displacement. Hence, there can be two directions or two planes of at movements which are normal to the propagation direction of the vector.

So, I have got longitudinal waves and I have got transverse waves and they are the phonons which can be called as acoustic phonons

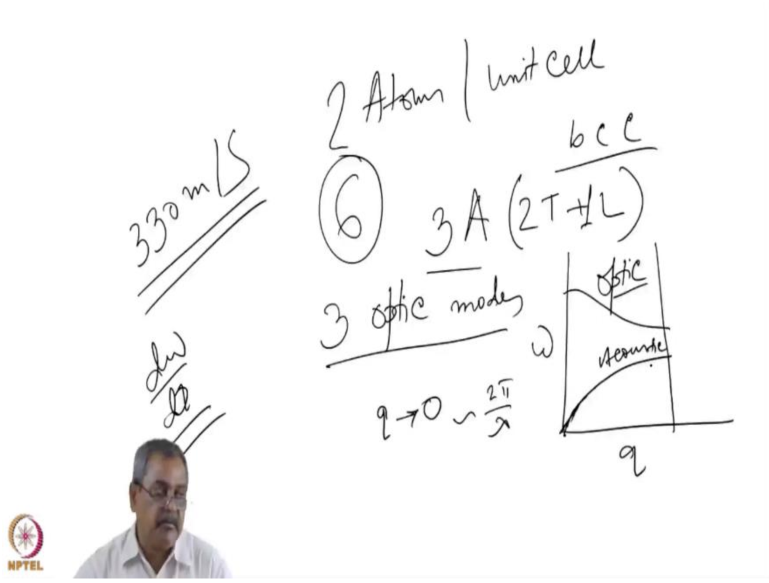
Let me just quickly tell you if there is only one atom per unit cell then there are three degrees of freedom. There will be one acoustic phonon mode where two of them will be transverse modes, as I told you earlier. If the propagation was parallel to the *z*- direction then one (transverse mode) can be in the *x* direction and other mode can be in the *y* direction. So, out of three acoustic modes, two are transverse and one is longitudinal where the displacement is along the propagation direction, say along *z* direction. So, I have got three acoustic modes which are possible when I have one atom per unit cell.

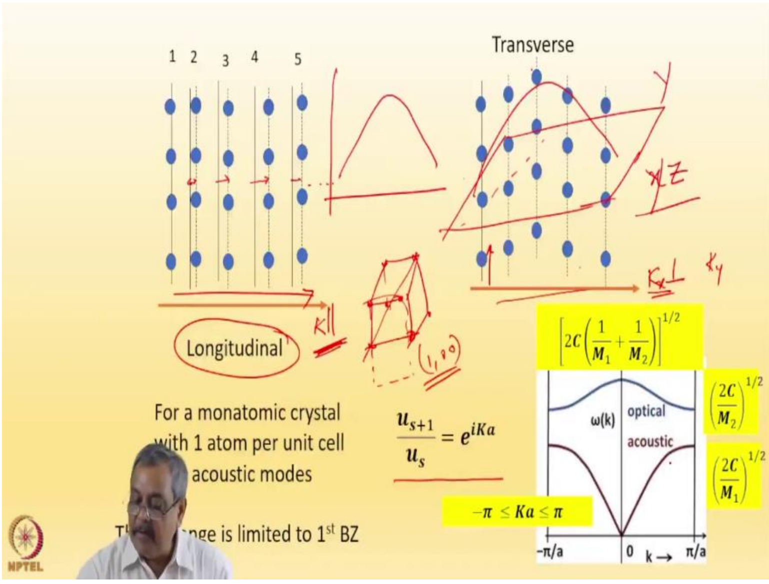
Another interesting aspect is that from the formula that we used the $\frac{u_{s+1}}{u_s} = e^{iKa}$, that means the neighboring atom displacement ratio is given by e^{iKa}. When $Ka = \pi$ then I have $\frac{u_{s+1}}{u_s} = e^{i\pi}$. means they are exactly out of phase with respect to each other. Now, say if $Ka = \pi + 0.2\pi$. This is something which I will try to explain to you. In case of a Brillouin zone, the zone boundary comes at π/a and $-\pi/a$. What is a Brillouin zone? I am showing you the reciprocal lattice space (of a square lattice) when the nearest neighbors are at a distance $2\pi/a$ because that is the reciprocal lattice vector when the real lattice vector is a. Then you draw a perpendicular bisector at π/a, same thing is true in the negative direction, and the bisector comes at $-\pi/a$. So $-\pi/a$ to $+\pi/a$ form the first Brillouin zone and when $K = \pi/a$ then I have reached the Brillouin zone boundary.

Now when I go to $K > \pi/a$, a point here, say greater by $0.2\pi/a$ then I can reflect it by $2\pi/a$ to minus $-0.8\pi/a$ so I can bring it back by reflection to the first Brillouin zone. Anything outside the first Brillouin zone, say in the second Brillouin zone can be reflected back to the first Brillouin zone. That means my dispersion relation of ω vs q is limited to the first Brillouin zone. I have drawn here the positive side of the first Brillouin zone, I can also draw the negative side but it will be just the mirror image of this one and anything beyond first Brillouin zone can be reflected back (to the first zone).

So, $Ka > \pi$ can be taken to $Ka < \pi$ just by reflection, and this is what is done in phonon studies.

(Refer Slide Time: 9:12)



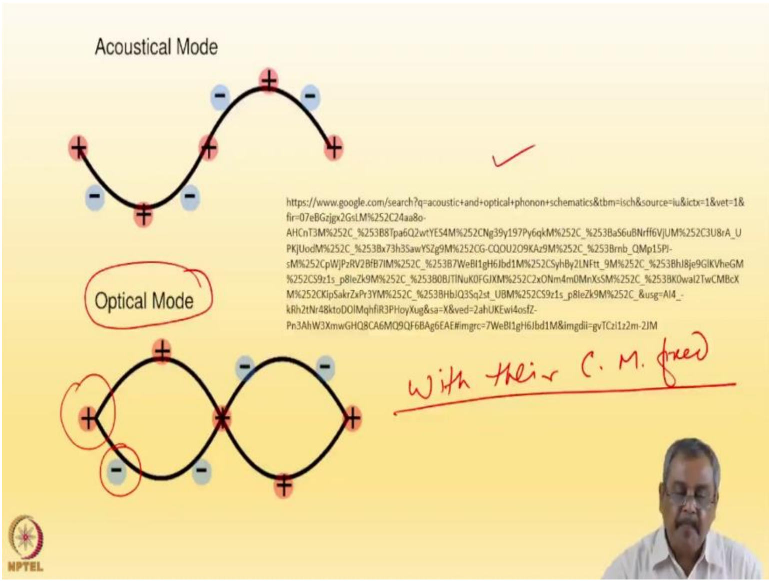


Now if there are more than one atom, suppose there are two atoms per unit cell, an ideal example would be a bcc lattice where we have one atom at the body center and there are 8 atoms at the corners (shared by 8 neighbors) coming to 1 atom (per unit cell) and resulting in 2 atoms per unit and you got 6 degrees of freedom. When you have 6 degrees of freedom you have got 3 acoustic modes including 2 transverse and 1 longitudinal. Then there will be 3 remaining modes what are known as optic modes.

The dispersion relation will also have branches known as optic branch. I will come to this later in little more detail. So, I have got optic branches and I have got acoustic branches. Why this is called acoustic branch! Because in this acoustic branch when q (=$2\pi/\lambda$ where λ is wavelength of the phonon tends to 0 or λ becomes long, enough, you go into sound limit and the dispersion becomes nearly linear.

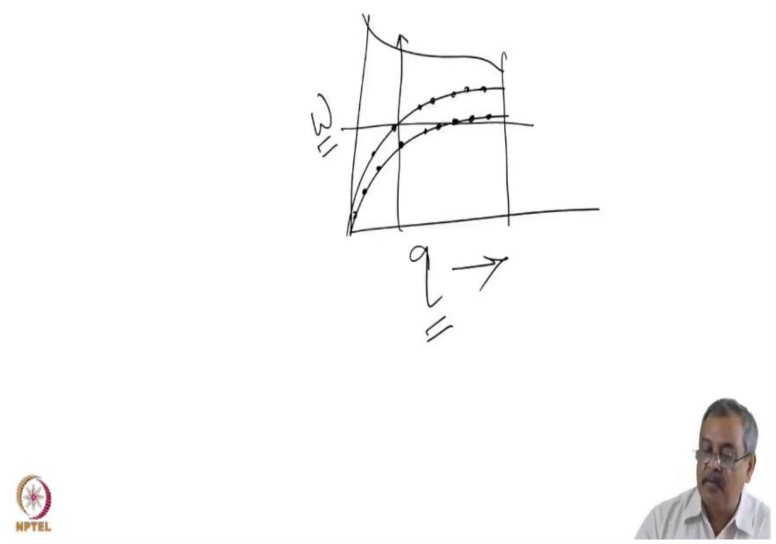
We know that the sound wave propagates with 330 m/sec velocity (in air) and here also you can calculate from $\frac{d\omega}{dq}$ that as q tends to 0 we will go to sound wave limit. but when we have shorter wavelengths or larger q values then they are the relative oscillations that propagate with different velocities. Their group velocities are different. Because of this q going to zero limit this is known as acoustic branch. I will come to the optical branch in the next lecture.

(Refer Slide Time: 11:26)



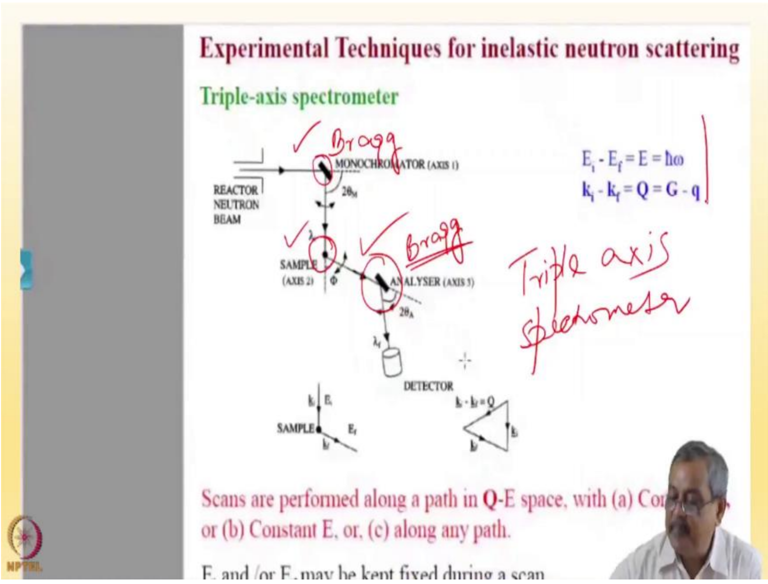
I talked about 3 acoustic modes, 2 transverse and 1 longitudinal, for any number of atoms and others are optical branches. In the acoustic mode, shown here, you can see that the movement of the points, such as atomic position in a crystalline lattice, If I am talking about aluminum phonons then these are the positions of the aluminum atoms at lattice points and their movements are like this. They are part of a wave and they move in the same direction. Whereas when I am talking about optical modes then they move against each other. These positive and negative symbols are not charges rather it shows that if an atom moves in a particular direction the nearest neighbor moves in the opposite direction. So, atoms are moving against each other with their center of mass fixed, in the optical modes. How to define optical modes? We will come to it later but this comes when you have got either two equivalent atoms in the unit cell or inequivalent atoms, if they are inequivalent atoms and if this positive and negative are the ionic charges for the lattice sites then you can see these movements of the atoms at the lattice side look like a dipole oscillating and it can absorb energy from an optical wave or it can give energy to an optical wave. That is why phonons with the atoms move against each other are known as optical modes and the dispersion relations are also different compared to the acoustic modes, I will come to this later. So, we have acoustic modes and optical modes and we need to do measurements of the dispersion relations (ω-q measurement).

(Refer Slide Time: 13:49)



I draw modes like this on ω *vs* q plot. I have to measure these points on the dispersion curve in $q\omega$-space. For this, we need to have instruments which can measure q and which can measure energy transfer and we should also be able to probe either along the constant q (vertical line in the plot)or along the constant ω (horizontal line) and every time we touch one of these dispersion curves we will get a peak because that is an allowed phonon and that energy transfer is allowed, so we have to design instruments to measure these changes.

(Refer Slide Time: 14:49)



I just show you the triple axis spectrometer at Dhruva. You can see this is the monochromator drum at the center of which we have the monochromator crystal (first axis), then we have a sample here on the rotating table (second axis) followed by another rotational stage on which you have an analyzer (third axis) and then a detector. So, the geometry of the experiment is like this, there is a monochromator which can rotate around its axis to change the incident energy. We have a sample which can rotate around its axis. If it is a single crystal then you can tailor scattering various atomic planes, using a goniometer on the sample table. And then you have an analyzer crystal here which analyzes the energy of the outgoing beam by Bragg reflection, so, this (monochromator) selects the energy of the incident beam by Bragg reflection and analyzer gives energy of the scattered beam again using Bragg reflection.

The analyzer rotates along with the detector in θ-2 θ mode and that is why it is called triple spectrometer because there is one axis for monochromator, second axis for the sampleand the third axis for energy analysis using the analyzer. Here we can measure the energy transfer and we can also measure the momentum transfer in a scattering experiment. I will come to this in greater details.

The first triple axis spectrometer was designed by Bertram Brockhouse at NRX reactor in Canada and he got the Nobel Prize for studies on dynamics of material. There are other instruments like filter detector spectrometers, spin echo spectrometers, I will touch upon all of these spectrometers that are used for inelastic neutron scattering.