Neutron Scattering for Condensed Matter Studies
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Week 02
Lecture 03B
Scattering theory and introducing dynamics in the formalism

Keywords: Nuclear Spin, Neutron spin, Coherent scattering cross-section, Incoherent Scattering cross-section

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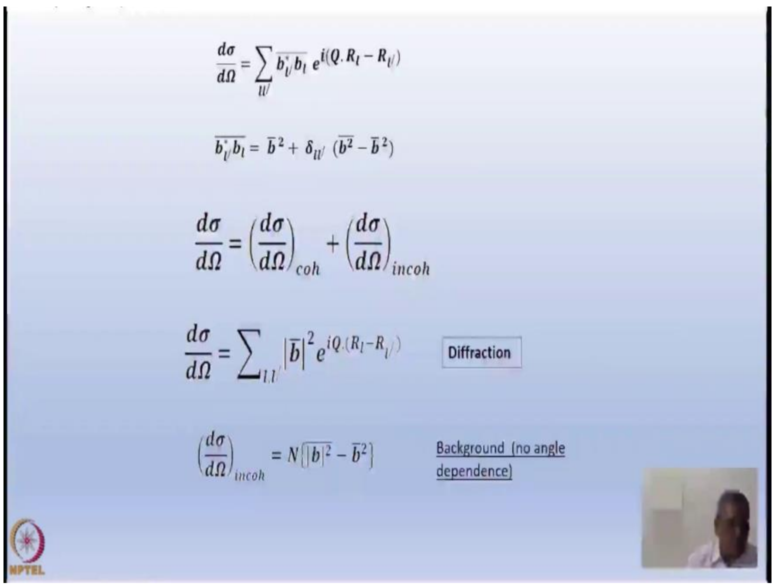

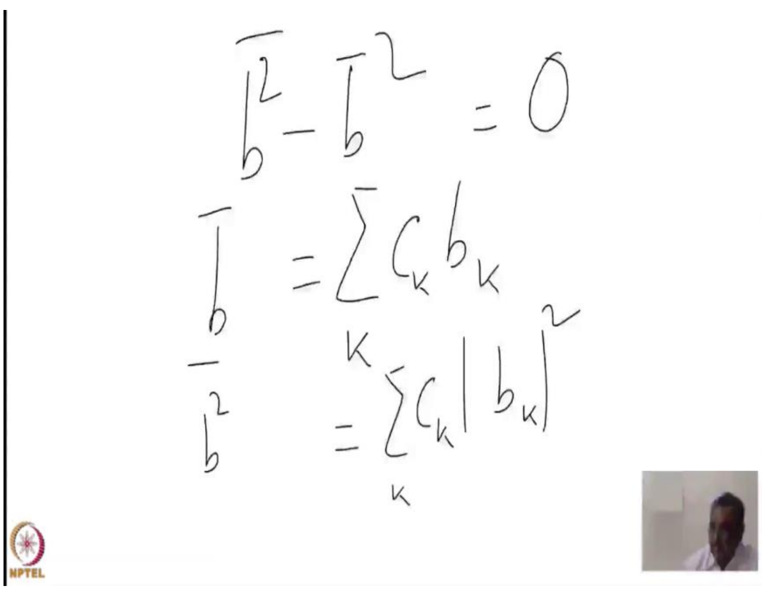

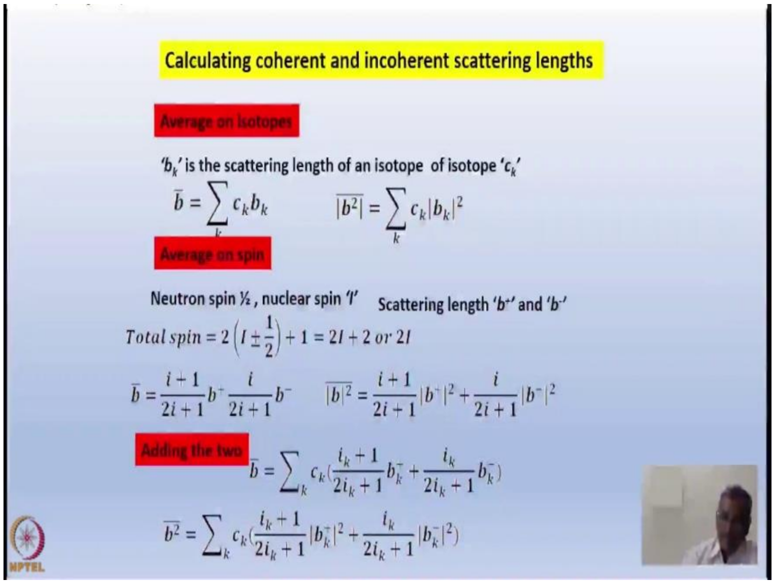

I have two terms now in neutron scattering, this fluctuation term is 0 for x-rays. Hence, if I consider some scattering length for x-rays, it is same everywhere and there is no fluctuation and there is no incoherent scattering. But in case of neutrons, it is not so and now I will go ahead and show you how to tackle it.

We can experimentally find out that the scattering length of an isotope 'k' which has got a concentration c_k, then the average depends on the concentration and it is simply $c_k b_k$, if b_k is the scattering cross section of one isotope with concentration c_k then considering all scatterers (isotopes) in the entire sample, $\bar{b} = \sum_k c_k b_k$. Similarly, the b square average is nothing but if the b_k is the scattering length for an isotope with concentration c_k then it is, $\overline{b^2} = \sum_k c_k |b_k|^2$.

So, b average is nothing but concentration c_k of an isotope and its scattering then b_k, and b square average is equal to same sum on the square of that. I can calculate the diffraction from this. I will talk about the spin now.

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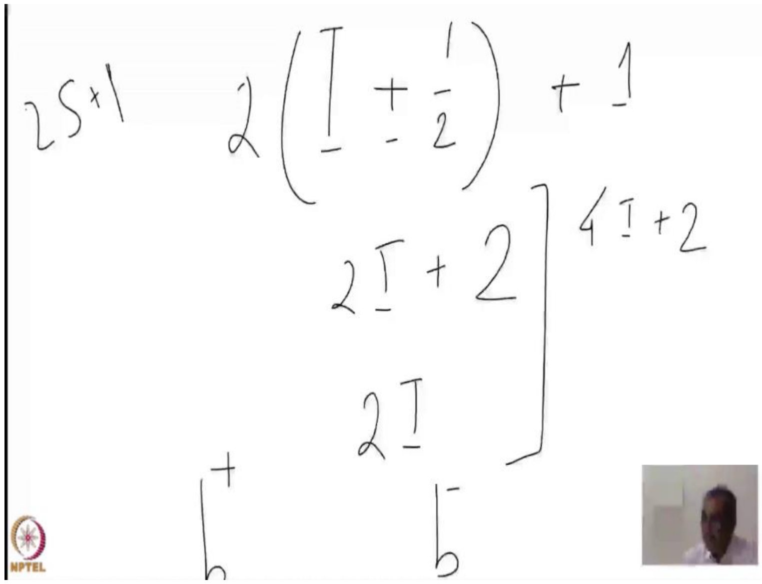

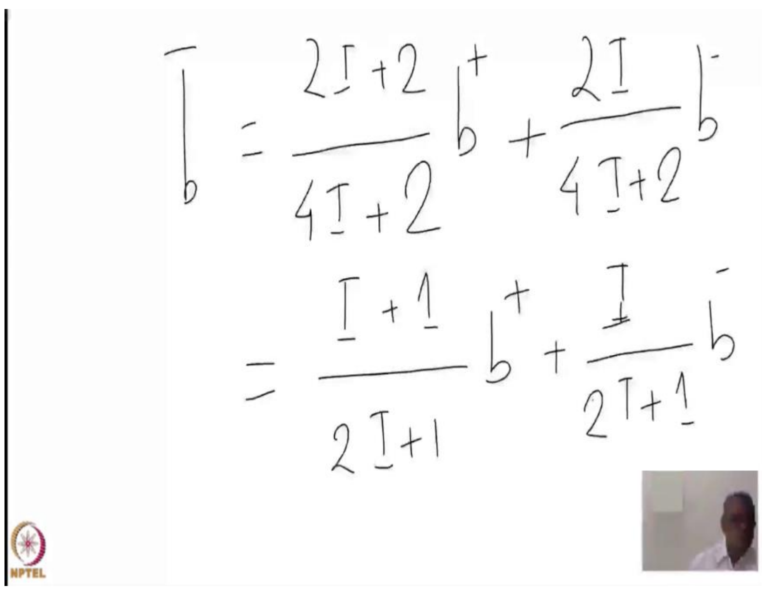

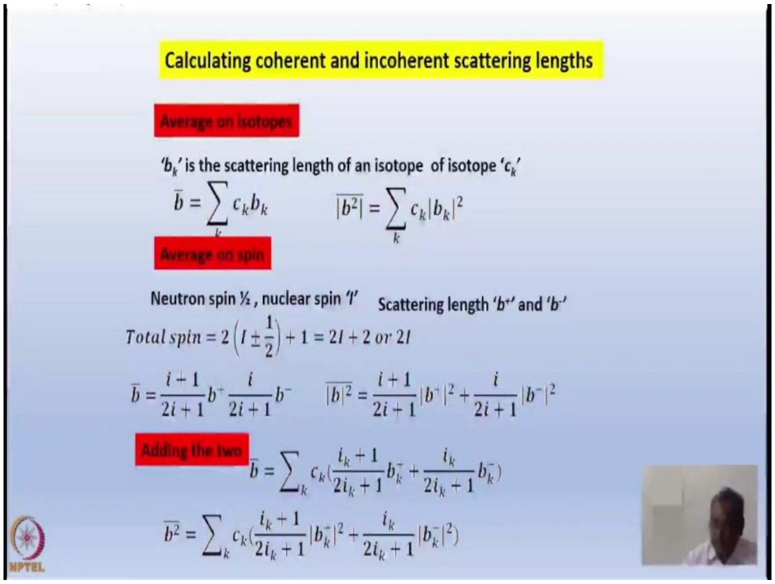

In case of spin, suppose the nucleus has a spin I and the neutron has a spin 1/2 so we know from quantum mechanics 2S+1 are the possible states. So, for neutron-nucleus system total spin is 2(I ±1/2) + 1, nuclear spin (I) is either parallel to neutron or antiparallel. For plus sign, total value is 2I + 2 and for minus sign it is 2I. Hence, there are 4I + 2 possibilities.

In summary, when nuclear and neutron spins are parallel then the possible states spin states are 2I + 2, while when they are anti-parallel the possible spin states are 2I and these are the weight factors. When they are parallel let us consider the scattering length is b^+ and when anti-parallel let us call it b^-. Then, the weightage for b^+ will be $\frac{2I+2}{4I+2}$ and for b^- will be $\frac{2I}{4I+2}$. Hence $\bar{b} = \frac{2I+2}{4I+2}\ b^+ + \frac{2I}{4I+2}\ b^-$.

To find out b^+ and b^-, we have to do a very elaborate experiment, you have to make the neutron polarization parallel to the polarization of the nucleus and then we have to do it. But, right now, theoretically if this is the case then you have the averaging over the spin is given by

$$\bar{b} = \frac{I+1}{2I+1}\ b^+ + \frac{I}{2I+1}\ b^-$$

when the nuclear spin is I.

Now, we have the case where you have the isotopes and the spins.

If I consider an isotope, k^{th} isotope with nuclear spin I_k, and the concentration c_k then the expression for b average is,

$$\bar{b} = \sum_k c_k \left(\frac{I_k + 1}{2I_k + 1}\, b_k^+ + \frac{I_k}{2I_k + 1}\, b_k^- \right)$$

and in the same way the b square average is that only I put square of these terms and weightage are the same.

$$\overline{b^2} = \sum_k c_k \left(\frac{I_k + 1}{2I_k + 1}\, |b_k^+|^2 + \frac{I_k}{2I_k + 1}\, |b_k^-|^2 \right)$$

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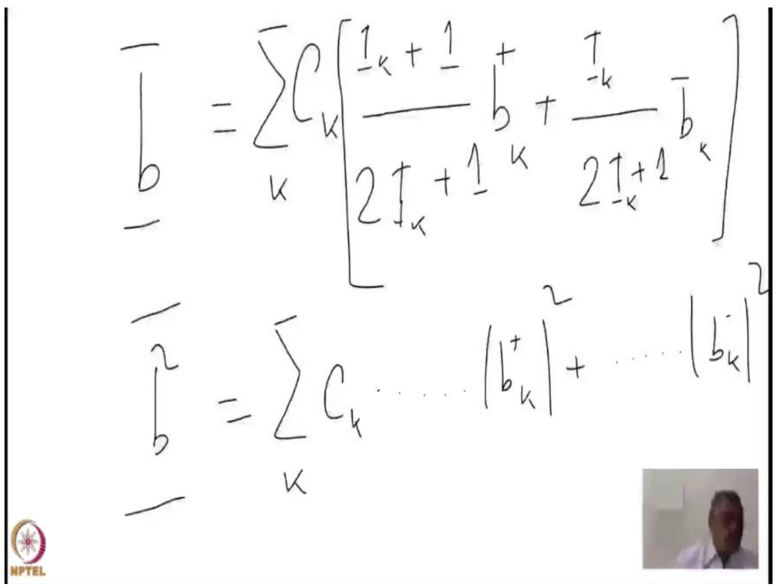

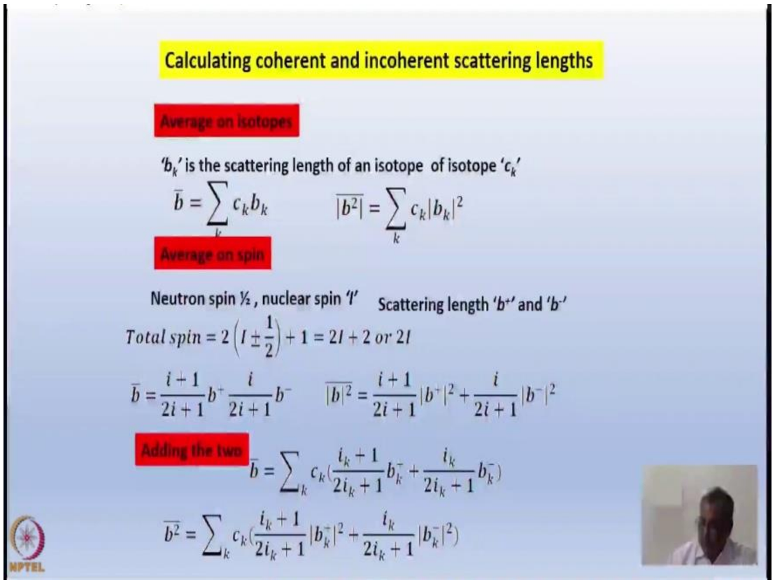

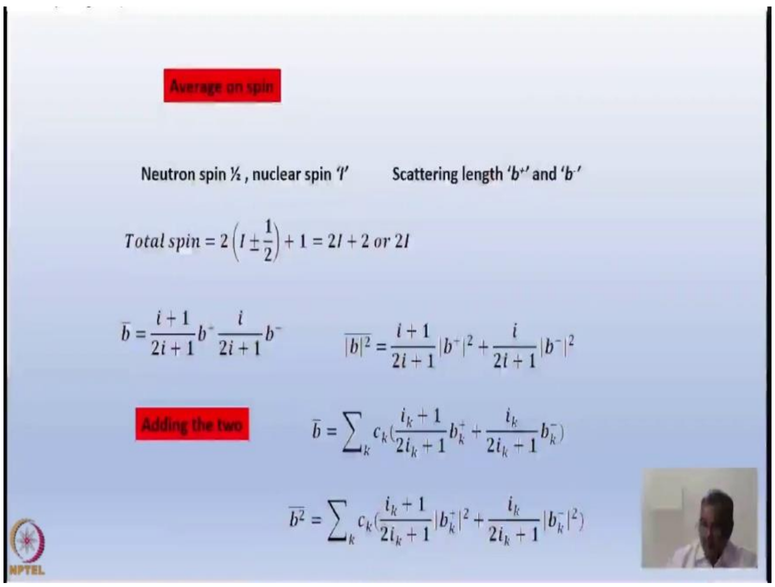

This way, one can calculate b average and b square average for a distribution of isotopes and spins with k^{th} isotope having concentration c_k and spin I_k. These are the expressions, adding the isotope and spin in a formalism.

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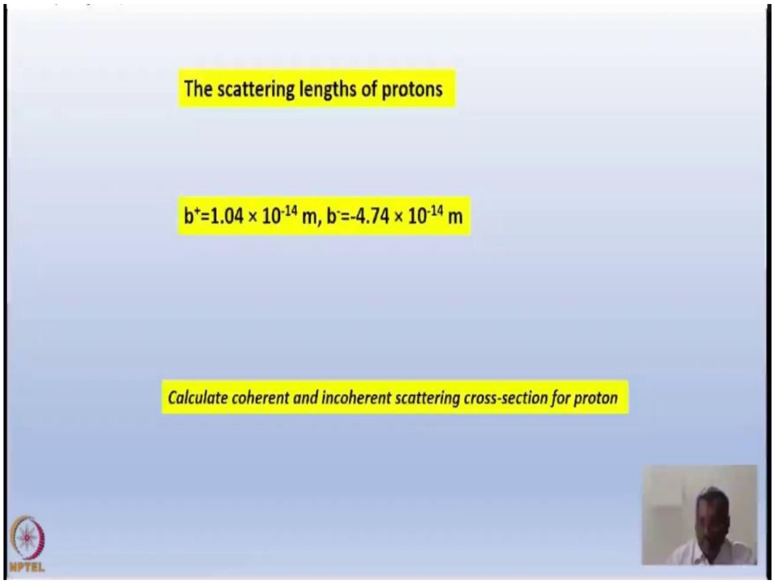

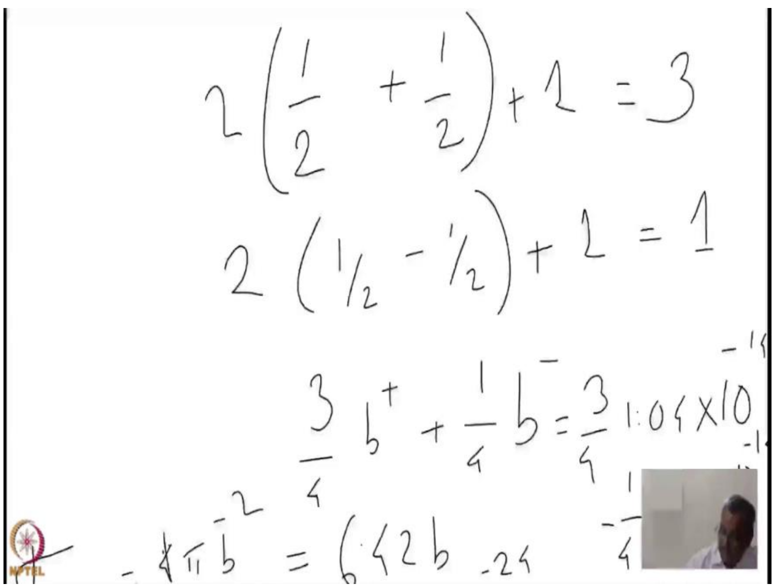

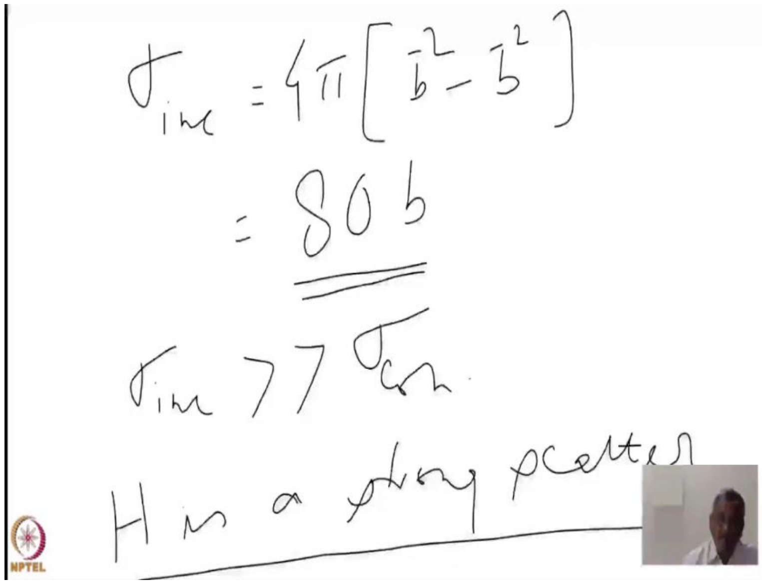

For example, the b^+ for the most common isotope which is hydrogen is 1.04×10^{-14} m and b^- is -4.74×10^{-14} m. I request you to calculate the coherent and incoherent scattering cross section for proton using these values, let me just do a few lines for you so that you become familiar with this.

It is the simplest calculation because proton has a spin 1/2, neutron has a spin 1/2, so 2I + 2 = 3 and 2I = 1. Hence, the spin weightages are 3 and 1. I am telling you to do the spin average scattering cross section, so what you need to do is actually is, $\frac{3}{4}\ b^{+} + \frac{1}{4}\ b^{-}$. Putting the values of b+ and b- for Hydrogen, $\bar{b} = \frac{3}{4} \times (1.04\ \times 10^{-14}) - \frac{1}{4} \times (4.74\ \times 10^{-14})$ m.

You can see that this is subtracting one term from another. Question comes how come a scattering length is negative! Right now, I will request you to accept it that in case of neutrons it is possible to have positive and negative scattering lengths because of certain nuclear constraints. Because of this you will find $\sigma_{coh} = 4\pi\bar{b}^2$ in this case (Hydrogen) will come out approximately 6.42 barns where 1 barn = 10^{-24} cm^2. And, the $\sigma_{inc} = 4\pi\left[\overline{b^2} - \bar{b}^2\right]$, for this you can evaluate b square average in the same way I did it and you will find it will be coming around 80 barns.

You can see that for hydrogen σ_{inc} (incoherent part) >> σ_{coh} (coherent part). It means hydrogen is a very strong scatterer, but it scatters incoherently. So, for a diffraction experiment hydrogen is not so suitable.

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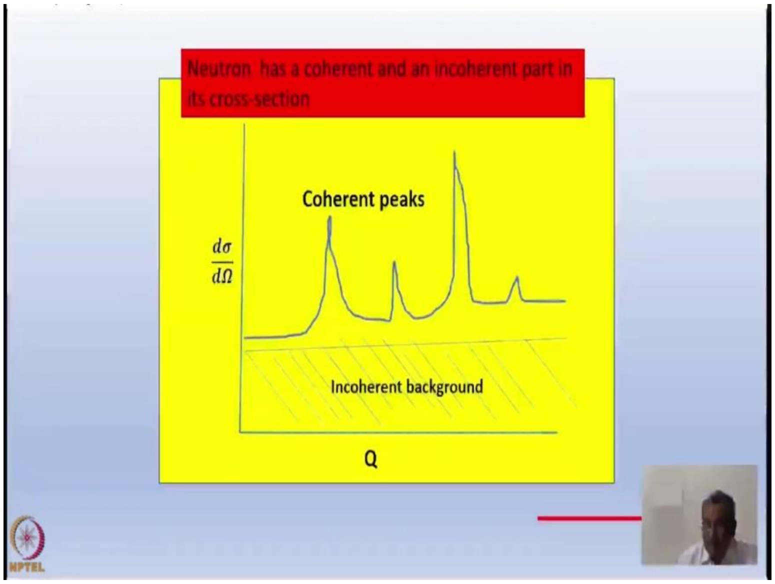
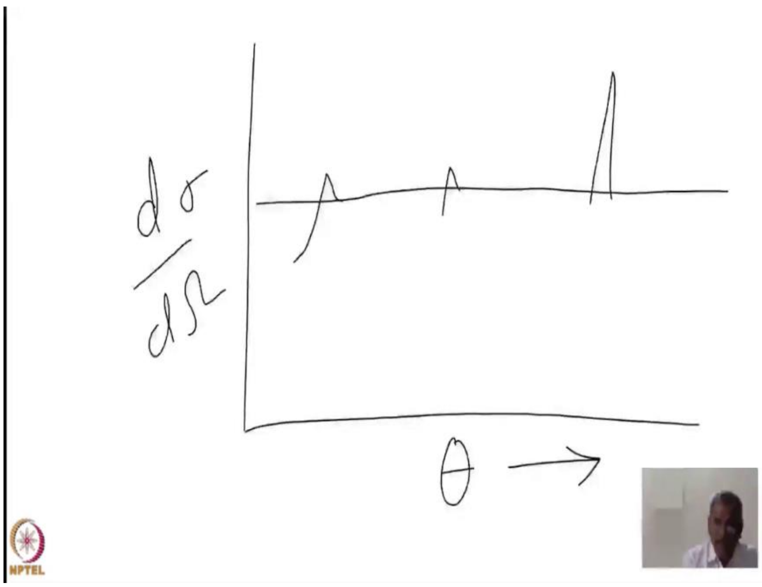
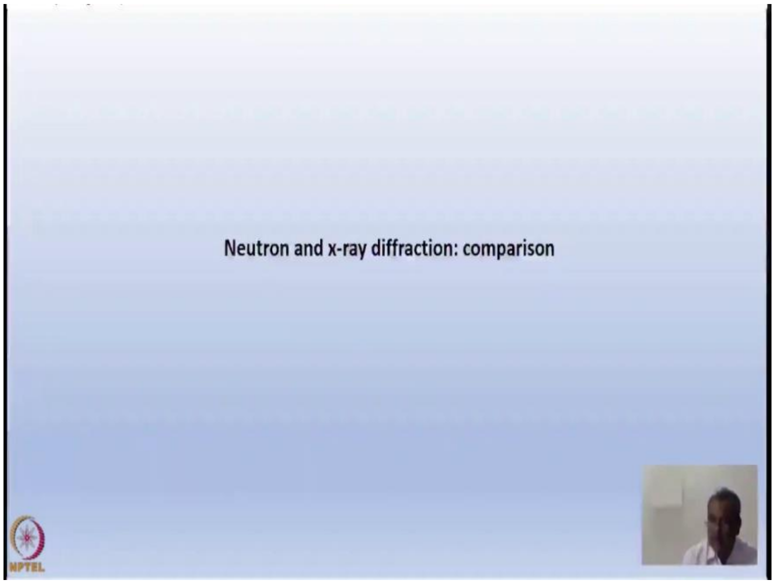

Neutron has a coherent and an incoherent part in its cross-section
Coherent peaks
$\frac{d\sigma}{d\Omega}$
Incoherent background
Q


$\frac{d\sigma}{d\Omega}$
$\theta \rightarrow$



I will just show you which is coherent and incoherent part. The coherent part as I am repeatedly telling you it has got $Q.(R_l-R_{l'})$ and if you do an experiment on a material with large coherent cross section then you will find the coherent peaks. But incoherent part does not have any angle dependence it gives an incoherent background.

Because of this if you use hydrogenous material, you will find that in your experiment you have got a very large background and possibly the coherent peaks are just about rising on top of them. This is a disadvantage of doing neutron diffraction experiments with hydrogen. It does not mean hydrogen is not used, it is also used in some of the scattering experiments and also some of you may be aware that H_2O is a very strong moderator because it very strongly scatters neutrons and thermal neutrons and can cause very efficient thermalization of neutrons because it has got a very large cross-section, which is around 80 barns.

With this I stop the module where I have introduced you to the coherent and in coherent scattering cross section for neutrons. In the next part, I will show you a comparison between neutrons and x-rays because x-rays are most commonly used microscopic probe and then I will stop today.