Neutron Scattering for Condensed Matter Studies

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Week 02
Lecture 03A
Scattering theory and introducing dynamics in the formalism

Keywords: Diffraction, Coherent Scattering Cross-section, Incoherent Scattering Cross-Section

In today's lecture, I will give you a brief recapitulation of what we did regarding the scattering cross section for diffraction of neutrons. We started with the Fermi Golden rule and then we went ahead and calculated the scattering amplitude, $f(K, K^{'})$ from either a single scattering object or an assembly of them.

I will go ahead and using the same formalism I will show you that for neutrons we have something called coherent and incoherent scattering cross section which is not there in x-rays and I will explain to you why they are not there. Then, I will also go for a comparison between x-rays and neutrons because, x-ray diffraction is the most commonly used tool by researchers in any field of condensed matter, be it physics, chemistry or material science. We will do a quick comparison and show you what are the similarities and the dissimilarities between neutron and x-ray diffraction. Please remember till now I am doing diffraction, that means, I am just trying to get the structure of a material using neutron diffraction.

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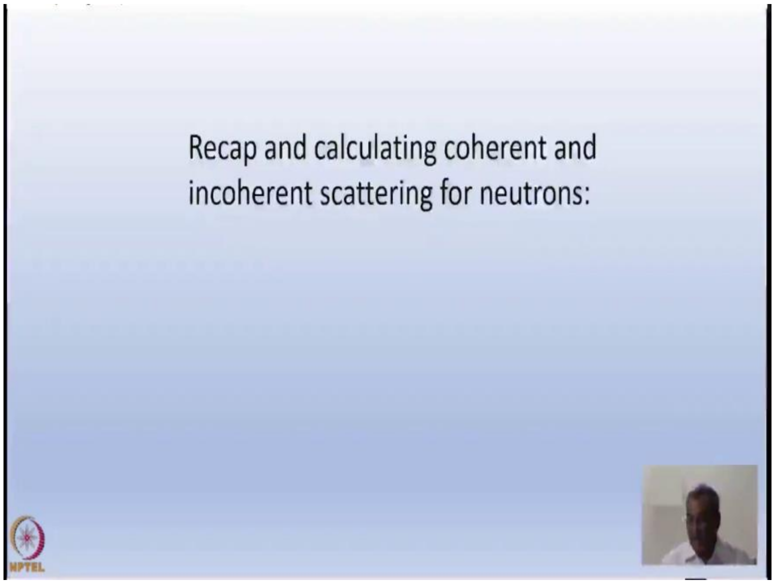

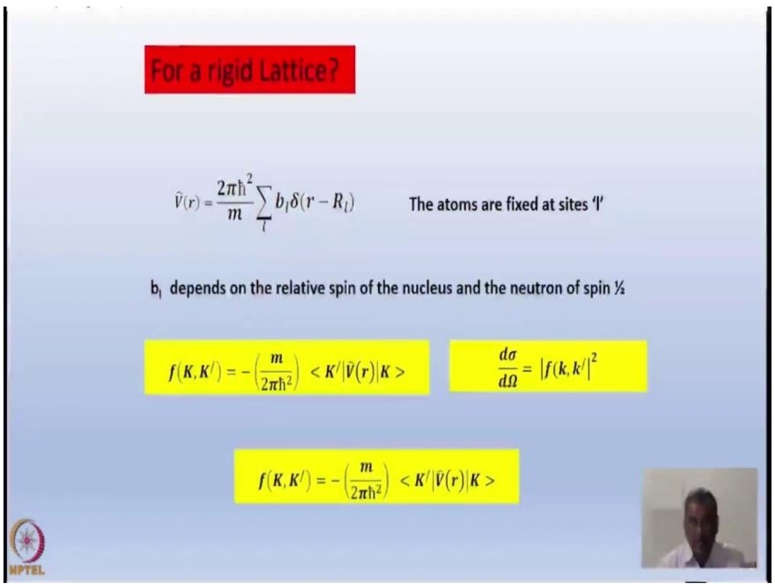

As indicated, recap and calculating coherent and incoherent scattering cross section for neutron will be our starting point for today's talk. Earlier also, I had written that for a rigid lattice. A rigid lattice means a lattice at 0 K so that I have a regular arrangement of atoms but they are rigidly fixed at their sites. I will come later what happens at finite temperature, so this rigid lattice I can consider as a sum of delta function potentials at site R_l and acting with a scattering amplitude b_l with the neutron.

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$$V(r) = \frac{2\pi\hbar^2}{m}\,\delta(r)$$

$$\lambda \gg r$$

$$V(r) = \frac{2\pi\hbar^2}{m}\sum_l \delta(\bar{r} - \bar{R}_l)$$

$$f(\bar{k}, \bar{k}') = -\frac{m}{2\pi\hbar^2}\langle k'|V|k\rangle$$

$$\frac{d\sigma}{d\Omega} = |f(k,k')|^2$$

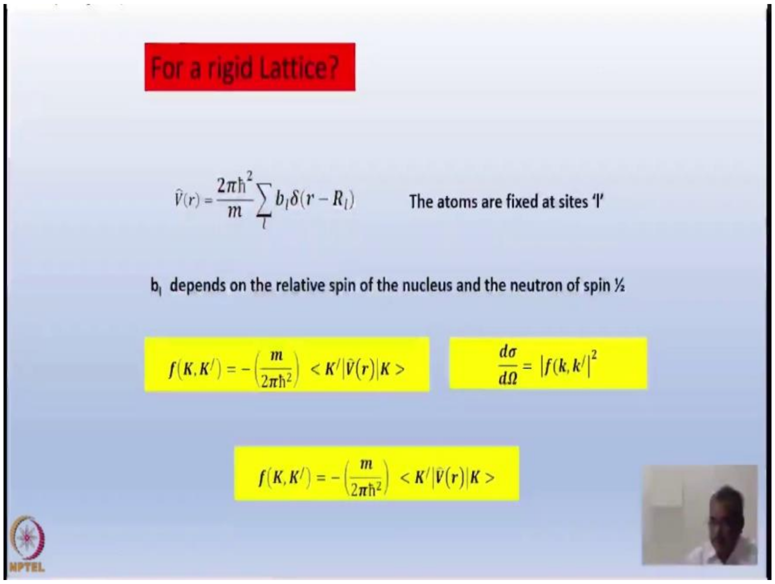
$$f(k,k') = \sum_l b_l\, e^{i\bar{Q}\cdot\bar{R}_l}$$

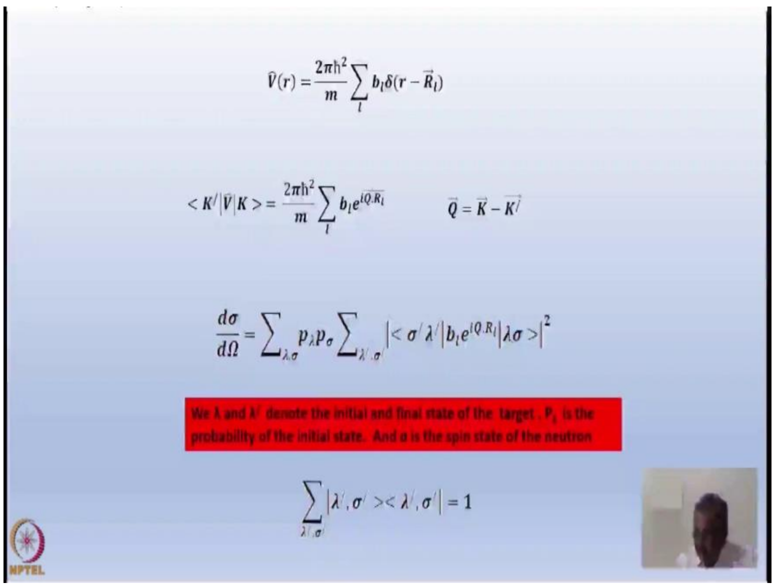
$$\bar{k} - \bar{k}' = Q$$

$$e^{i\bar{k}\cdot\bar{r}} \qquad e^{-i\bar{k}'\cdot r} \qquad e^{-i\bar{Q}\cdot\bar{R}}$$

$$\langle k'|\delta(r - R_l)|k\rangle$$

$$= \sum \int e^{i\bar{Q}\cdot\bar{r}}\,\delta(r - R_l) =$$





I had also given this delta function justification. I said that V(r), the scattering potential for a single nucleus, is a delta function because the nuclear potential is almost infinitely narrow with respect to the wavelength of neutron. So, wavelength of neutron is much greater than the nuclear radius. When I consider a lattice where the points are fixed in space then each of these points is a delta function. Now, I can write the V(r) is a sum of such delta functions; sum over all the lattice points. This was the potential offered by the entire lattice.

If you remember, the scattering amplitude f(K, K$^{'}$), when the neutron went from an initial wave vector K to the final wave vector K$^{'}$, was given by this. And $\frac{d\sigma}{d\Omega} = |f(K, K')|^2$ and you can see that there is $\frac{m}{2\pi\hbar^2}$ term in f(K, K$^{'}$). To cancel this term, I have put $\frac{2\pi\hbar^2}{m}$ in the potential.

Now with this let me just repeat the last equation. For a rigid lattice, I will be replacing the V by sum over δ functions and K – K` = Q. So, it goes to $\sum_l b_l e^{iQ.R_l}$ for the rigid lattice, it becomes a sum over all those delta functions and the delta function gives you, $\langle K'|\delta(r - R_l)|K\rangle = \sum_l \int e^{iQ.r} \ \delta(r - R_l)$, because $e^{iK.r}$ was the incident wave function and the outgoing wave function the complex conjugate was $e^{-iK'.r}$. When I put these two here, it gives me $e^{iQ.r}\delta(r - R_l)$ ultimately this along with the b, this integration becomes $\sum_l e^{iQ.r} \ \delta(r - R_l)$ and V also has this b part. This is what I showed for the scattering amplitude part.

So, this is what it was and $\frac{d\sigma}{d\Omega}$ is the square of that expression as I defined and $\langle K'|V|K\rangle = \frac{2\pi\hbar^2}{m}\sum_l b_l e^{iQ.r}$ where Q = K-K` as I derived for you. Now the system is in some initial state which is not just its momentum but the scatterer distribution, here I have to consider the distribution of the isotopes and also distribution of the spins. Why?

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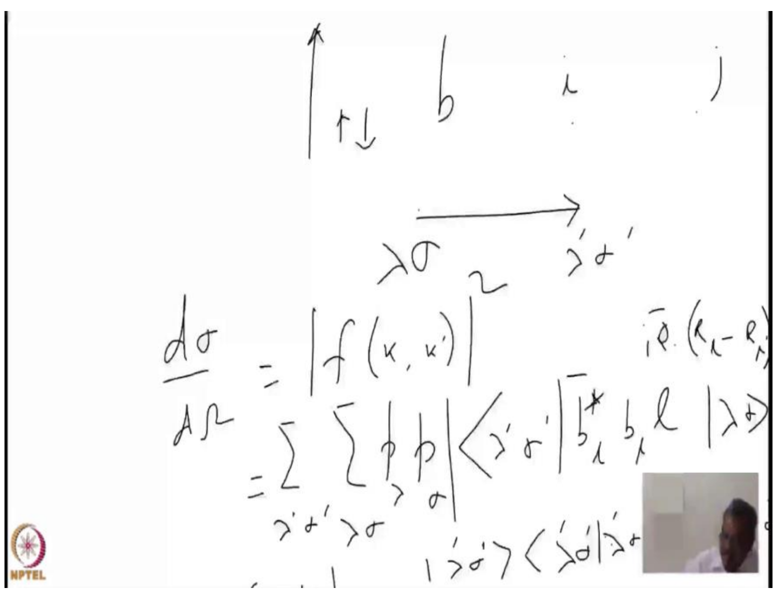

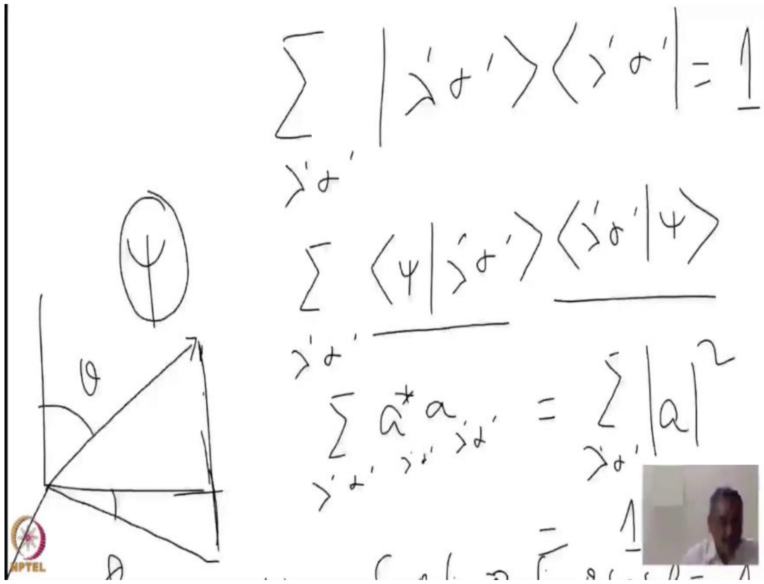

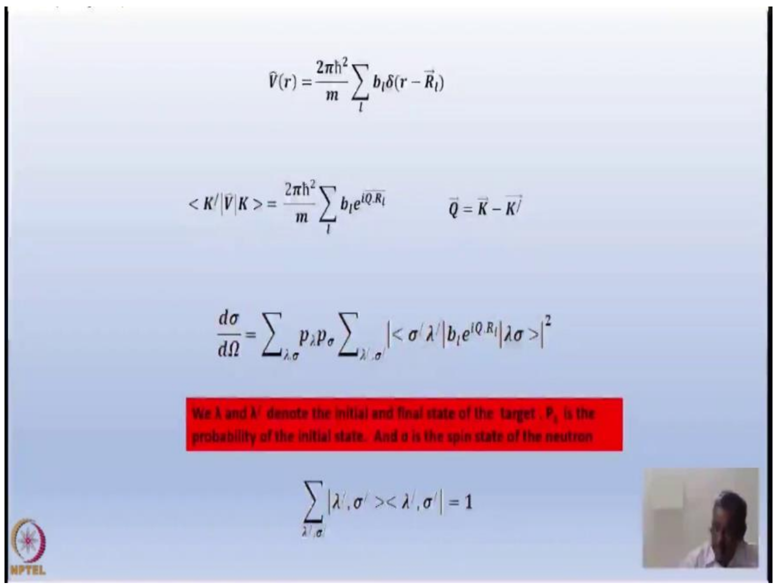

Because one is that nuclear spin and neutron spin, whether they are parallel or antiparallel, the value of b changes and also it changes from one isotope i to another isotope j. They are distributed all over the crystal and we assume that the nuclear spins are reorienting, it is a very reasonable assumption because it is difficult to align all the nuclear spins and at any instant the nuclear spin can be either parallel or anti-parallel. The isotope is also randomly distributed on the sites independently, one isotope position is independent of the other except statistically it is just given by the probability.

Now, imagine your system is in a state $\lambda\sigma$ spin and isotope and the final is one of the $\lambda'\sigma'$ states. I can do a summation over all possible initial states, when I do a squaring of it then what I have actually showed you, $\frac{d\sigma}{d\Omega} = |f(K, K')|^2$, modulus means f(K, K`) and its complex conjugate and it comes out like this.

Now, I have to do a summation over the final states, over all the initial states and I need to take the probability of all the initial states, then you have the complex conjugate and I have to square this whole thing. This is my scattering amplitude but you need solid angle. In this I have summation over $\lambda'\sigma'$ and I and I also have summation over $\lambda\sigma$.

I will just write briefly, I have $< \lambda'\sigma'|$ something and $|\lambda\sigma >$ then again there will be $<\lambda\sigma|$ $< \lambda\sigma|$then again one more bracket with $< \lambda'\sigma'|$ then ultimately you will have $|\lambda\sigma >$. Now, I can play with this. I am slightly wrong here, it will be sum over $\lambda\sigma$ then here it will be $\lambda'\sigma'$ then $\lambda\sigma$.

Now, I have a summation over $\lambda'\sigma'$ over the final states. This is a projection operator, why, let me just explain to you in more details. Suppose, I have a state function ψ in quantum mechanics now I want to know what are the components in these states, $\lambda'\sigma'$component of this. So, I can write it like this.

Now this bracket gives me the component of ψ along $\lambda'\sigma'$and this is a complex conjugate of that component. If I call it the probability amplitude *a* that this sum over $\lambda'\sigma'$ is nothing but is a summation over all values of a^*a, which is nothing but the sum of the probabilities over all the final states and that must be equal to 1. Because if I sum all the components of a wave vector along this, it is just like if I have a vector in three-dimensional space, if I sum over the thetas in all directions for that, all the direction cosines if I add up then it will be $\cos\theta$, $\sin\theta \sin\phi$ and $\sin\theta \cos\phi$, if I square then add them up it will be $\cos^2\theta + \sin^2\theta \sin^2\phi + \sin^2\theta \cos^2\phi = \cos^2\theta + \sin^2\theta = 1$.

It is the same thing in the wave vector space and that is why we put $\lambda'\sigma'$ $|\lambda\sigma >$ if I consider transition probability to all the final states, they will go to 1. I have put this probability sum equal to 1, I showed you why.

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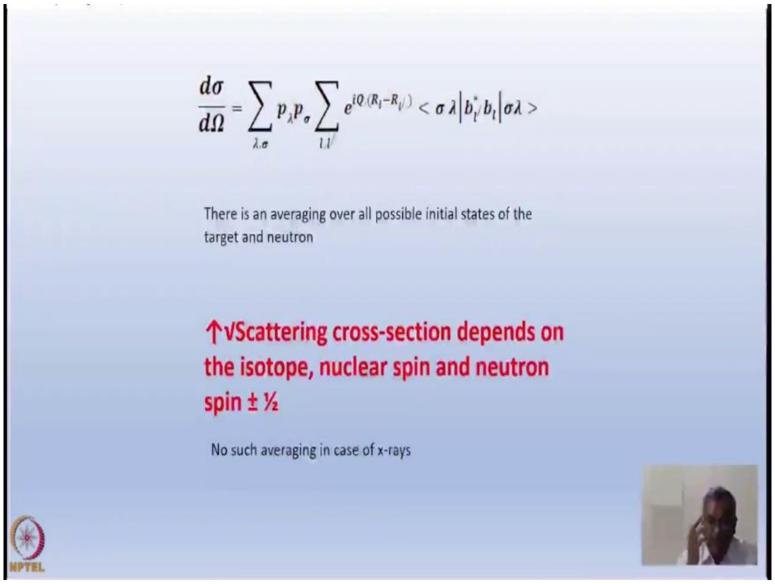

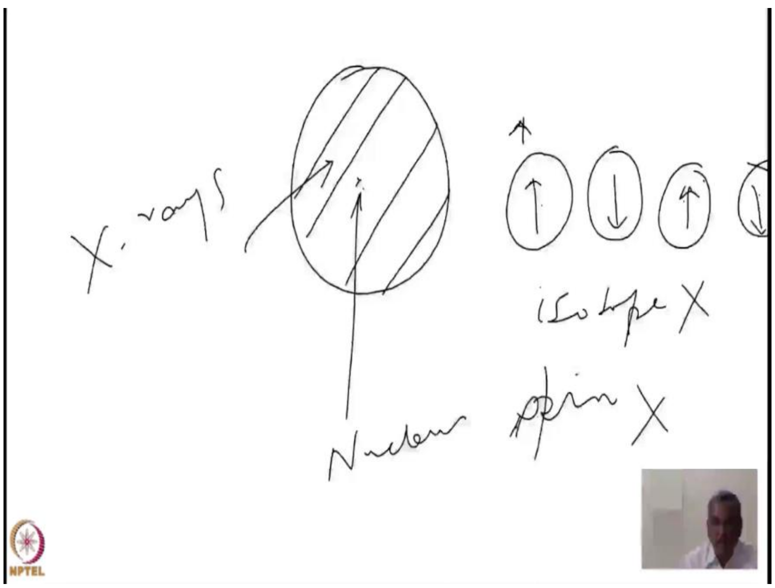

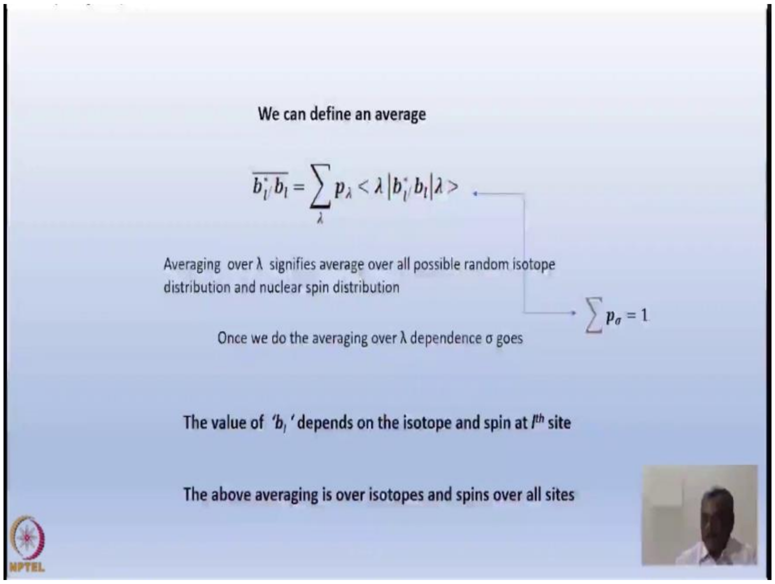

The scattering cross section per unit solid angle is given by, sum over all the initial states $e^{iQ.(R_l - R_{l'})}$ that came from the potential which is $\delta(r - R_l)$. There are two parts of it, there are two dummy variables 'l' and l' so it comes towards sum over ll' and that is averaging over σλ. It means I have to average the value of $b_l^{*}b_l$ over all possible initial states of target and neutron.

This brings a difference between neutrons and x-rays. Because scattering cross section here depends on the spin and the isotope, whereas if you are looking at diffraction pattern of x-rays from aluminum (just as an example) or any other metal, now aluminum has got a charge cloud which scatters and has a nucleus.

In this case, in the diffraction experiment my interaction of the neutron is with the nucleus and the x-rays are getting scattered from the charge cloud and the charge clouds, if I consider a lattice of aluminum, are same, charged cloud everywhere does not depend on the isotope or spin. That is why, in case of x-rays we do not have any averaging process whereas in case of neutrons we do have an averaging process which we will be using to calculate coherent cross section and incoherent cross section.

I will do the mathematics now but before that let me tell you the cause of this fluctuation is that in case of neutrons, first the nuclear spins are not oriented and the neutron spin can be either parallel or antiparallel to the nuclear spin and then the scattering cross section is different, so is the cause of the isotopes, the scattering cross section varies from isotope to isotope and you have to take an averaging on that also. It gives me an average scattering cross section and the fluctuation around them. Before I do the mathematics, that is the biggest difference between neutron and x-rays diffraction.

Now let me go ahead and calculate it. As I said that there is an averaging involved between the initial states for $b_l b_{l'}$ so here this is the average value. If I take sum over all possible spin orientation as one then it is all possible initial states p_λ, λ, $b_{l'}^* b_l$, λ so I have to do the averaging over all possible random isotope and nuclear spin distribution. Now let me try to write down this average value.

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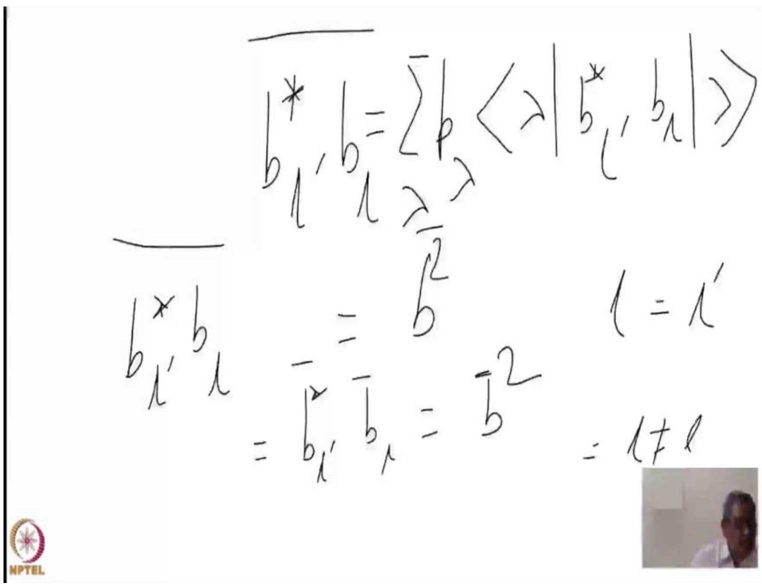

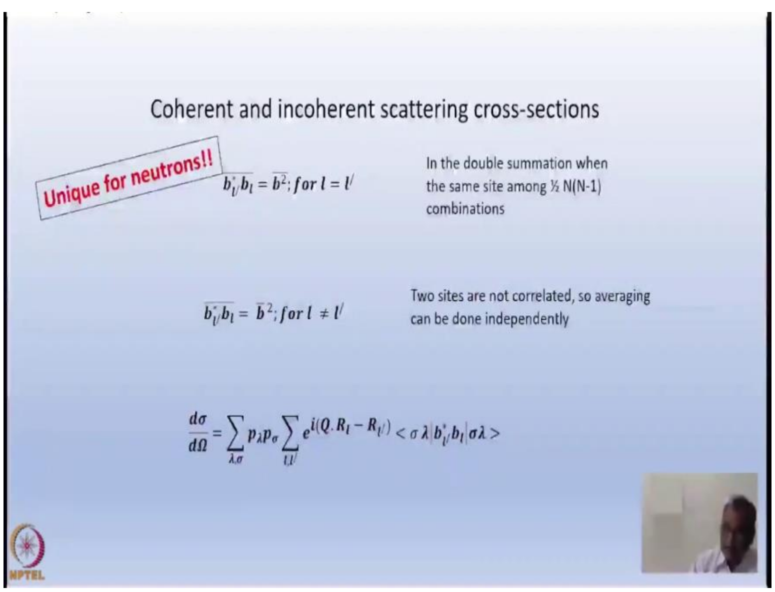

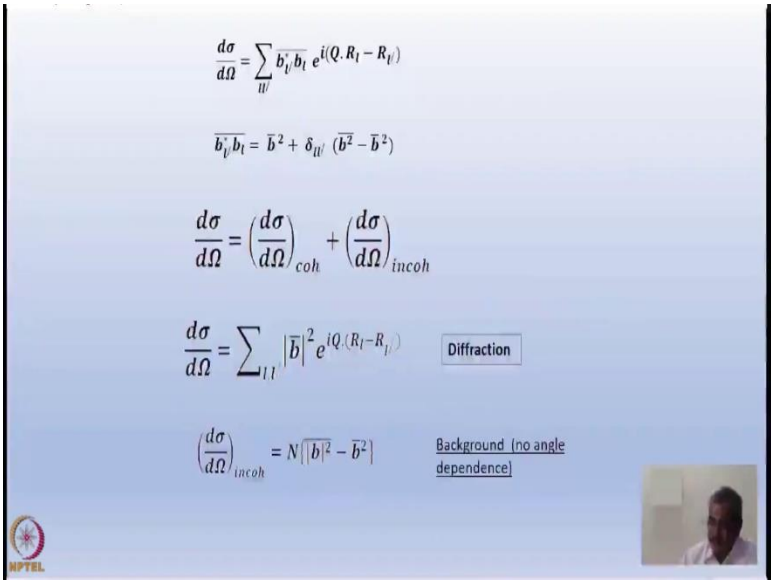

I have this at the l' site, the scattering cross section is $b_{l'}$ and its complex conjugate is $b_{l'}^*$ and I am doing an averaging over all the possible initial states which is also I have to put in. This, I will come to later. Now, in this averaging. There are two parts.

When $l = l'$ then, these two are same and what I get is $\overline{b^2}$ and I have to average of this. When $l \neq l'$ then you have to do the averaging separately because our assumption is that two sites are uncorrelated so far as their isotopes and spins are concerned.

I can do the averaging separately; two independent values can be averaged independently. This will also give me an average value b average star, so ultimately, I will have b average and square of that. So, I have two values when $l \neq l'$ and $l \neq l'$ and with this I get $\overline{b^2}$average and $\bar{b}^2$.

So, if the sites are not correlated the averaging is done separately. Now, in this summation, this averaging was there and now let me write it down in an interesting way.

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$$Q = \frac{4\pi}{\lambda}\sin\theta \qquad \overline{b^*_{l'} b_l} = \bar{b}^2 + \delta_{ll'}\left(\overline{b^2} - \bar{b}^2\right)$$

$\overline{b^2} \rightarrow$ Diff

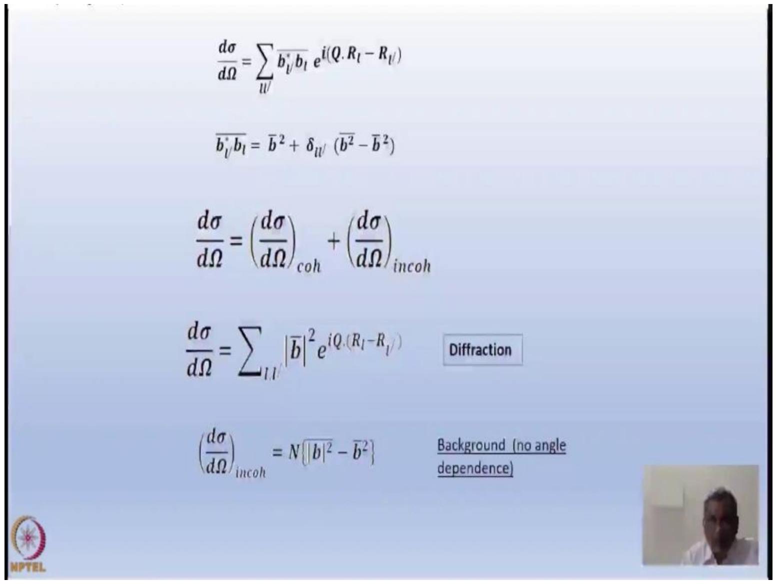
$$\frac{d\sigma}{d\Omega} = \sum_{ll'} \bar{b}^2 e^{iQ\cdot(\bar{R}_l - \bar{R}_{l'})} \rightarrow \text{Angle dependence}$$

$$+ N\left(\overline{b^2} - \bar{b}^2\right)$$

$$\overline{b^*_{l'} b_l} = \sum_\lambda p_\lambda \langle \lambda | b^*_{l'} b_l | \lambda \rangle$$

$$\overline{b^*_{l'} b_l} = \overline{b^2} \qquad l = l'$$

$$= \bar{b}^*_{l'} \bar{b}_l = \bar{b}^2 \qquad l \neq l'$$



I will write $\overline{b_{l'}^* b_l} = \bar{b}^2 + \delta_{ll'}\,(\overline{b^2} - \bar{b}^2)$.

I want to show you what I wrote actually this is equal to b square average ($\overline{b^2}$) when $l \neq l'$ and when $l \neq l'$ ` it is b square average ($\bar{b}^2$). These two statements I have absorbed in one expression.

You can see when $l \neq l'$ this term is 0 and I have b average square so that means distinct sites when they come into picture in this averaging, I have b average square and other part is not there. When $l = l'$ then this is 1 so b square average minus b average square these two cancels and I am left with b square average. There are two parts in this averaging, b average square and b square average.

Please note that when $l \neq l'$, scattering cross section is sum over ll' b average square $e^{iQ.(R_l - R_{l'})}$. $\frac{d\sigma}{d\Omega}$ scattering cross section per unit solid angle has two parts, one is when l in that summation not equal to l`, I have $e^{iQ.(R_l - R_{l'})}$ into b average square and another part when $l = l'$I have b square average minus b average square and sum over ll'. It will just give me N, number of lattice sides in the crystal.

Now please note that in $Q.(R_l - R_{l'})$, $(R_l - R_{l'})$ is the distance between the 'l' and 'l'' site and Q is the transfer vector. This has got an angle dependence and look at this term it does not have any angle dependence because there is no Q which is $\frac{4\pi \sin\theta}{\lambda}$,in magnitude and the direction is dictating what is the value of $Q.(R_l - R_{l'})$. This has angle dependence and other one does not have any angle dependence; the term b average dictates diffraction and this term does not have any angle dependence this acts as a background to the diffraction.

So now after deriving, you can see that this part is the incoherent part because it does not have any angle dependence and it depends on the fluctuation around the mean. b square average minus b average square is the fluctuation around the mean value of the scattering length at a site and the average value of the scattering length that are averaged over all the isotopes and spins gives me the diffraction term.