Neutron Scattering for Condensed Matter Studies

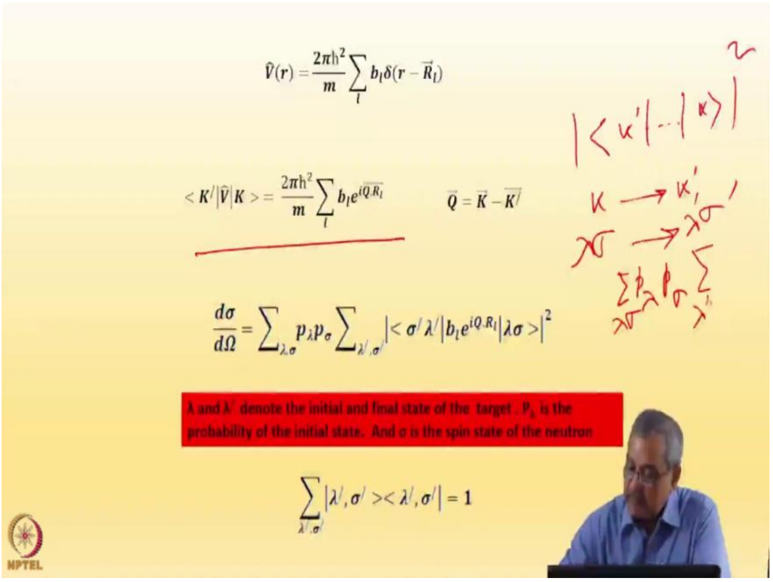
Professor Saibal Basu
Department of Physics
Homi Bhabha National Institute

Week 01: Lecture O2B

Deriving neutron scattering cross-section

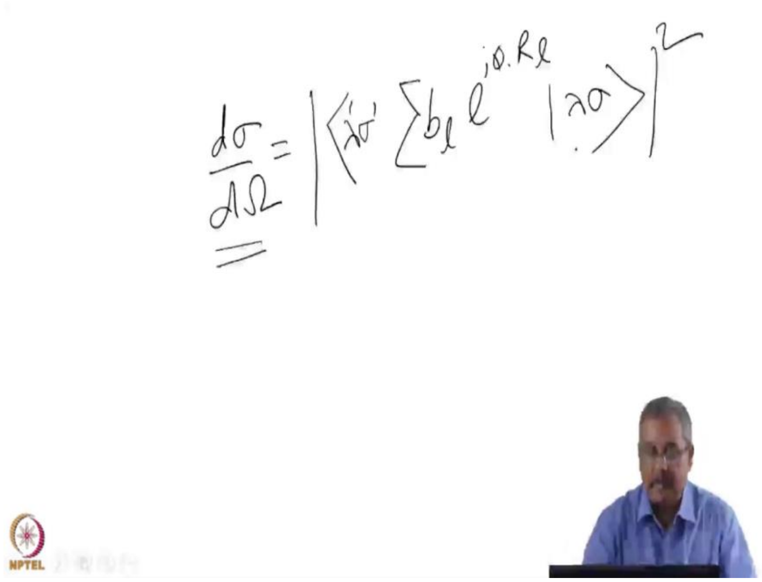
Keywords: Coherent Scattering Length, Incoherent scattering length, Neutron Diffraction, X-ray diffraction, Form factor

(Refer Slide Time: 00:14)



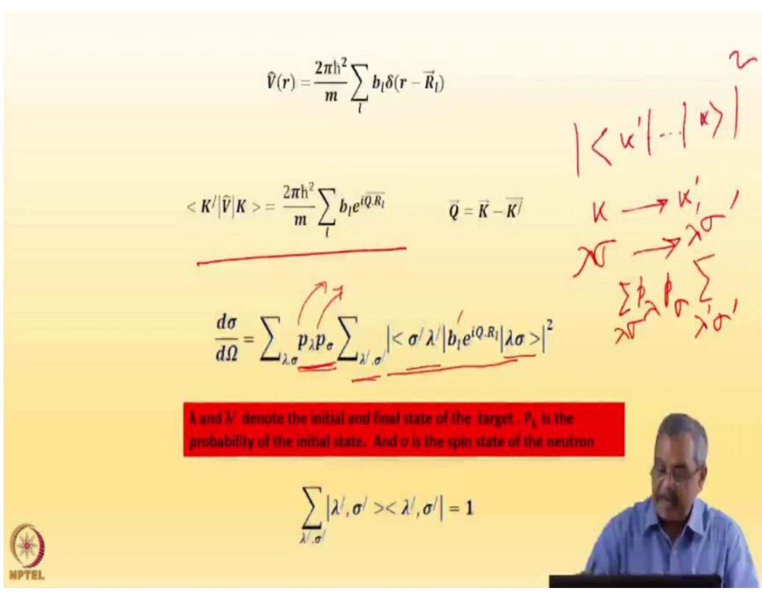
Now, when I consider the whole system there is a distribution of the initial states, so, I have to do it between K', potential and K and I have to square it ($|<K'|V|K>|^2$). Now, the thing is that K-K' = Q gives me $e^{-iQ.R_l}$ here, but now, I have a squaring to do and also, I have to do a statistical averaging, because, not only that it goes from K to K', if the initial state was λ and the neutrons spin was σ it also goes from λσ to λ'σ'. I have to do a summation over all the initial states with the respective probabilities and also sum over all the final states.

(Refer Slide Time: 01:21)



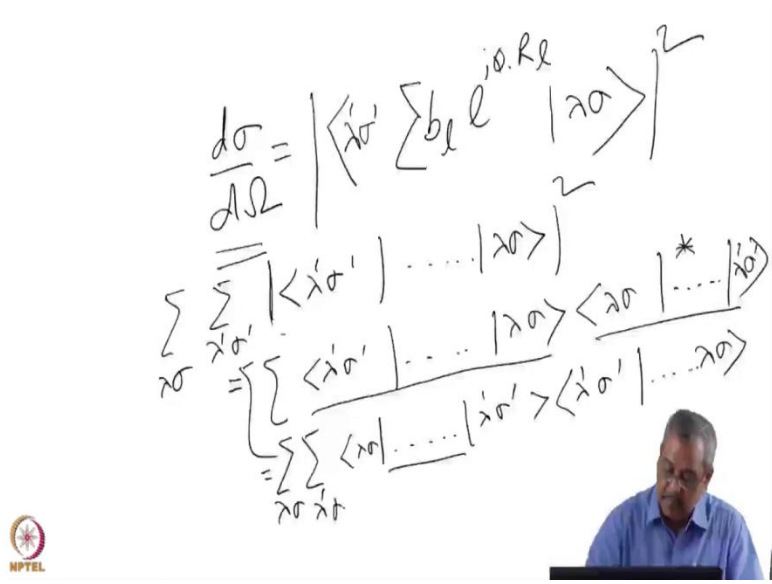
Let me say once again that $\frac{d\sigma}{d\Omega}$ will be given by a squaring of $\sum_l b_l e^{iQ.R_l}$ (this is the summation), here, I have taken care of K-K`, but I am doing it because it is going from some initial state to final state (λσ to λ'σ') where λσ includes energy spin (everything and λ'σ' also includes energy spin (everything) in the final state. And now, I have to square this because a square of this gives me $\frac{d\sigma}{d\Omega}$ the scattering cross-section, square of the scattering amplitude.

(Refer Slide Time: 02:25)



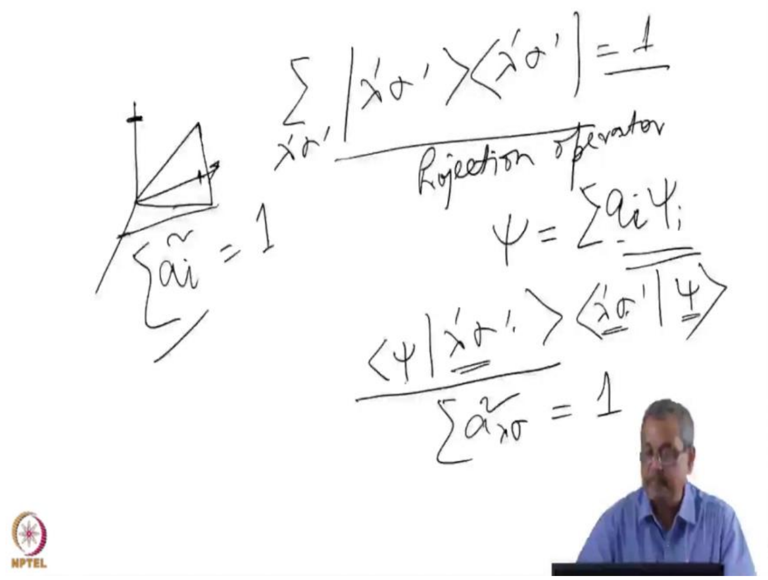
This is what I wrote here. So, it ($\sigma'\lambda'$) is the final state and ($\lambda\sigma$) is the initial state, then p_λ p_σ are the all probabilities of initial states of spin energy or anything else, e.g., isotope. Now, you can ask why I have not put p_λ $p_{\sigma`}$, because this expression gives me probability of all initial states, then the probability of transition from the initial state to all possible final states takes care of all the probabilities and that is why there is only $p_{\lambda`}$ $p_{\sigma`}$, just summation over all the final states and probability of all the initial state, but now, this bracket I can move around.

(Refer Slide Time: 03:16)



See these are separated wave functions. So, then here it will complex conjugate to be 'l'' $\lambda`\sigma`$, and now, I can move them around. I can write this equal to the summation (double summation remains) and like I can write it equal to $\lambda\sigma$ $\lambda'\sigma'$. If I bring this bracket to this side then I have $< \lambda'\sigma'|\ldots\ldots|\lambda\sigma >< \lambda\sigma|\ldots\ldots|\lambda'\sigma' >$, I have summation over $\lambda\sigma$ and $\lambda`\sigma`$.

(Refer Slide Time: 05:07)

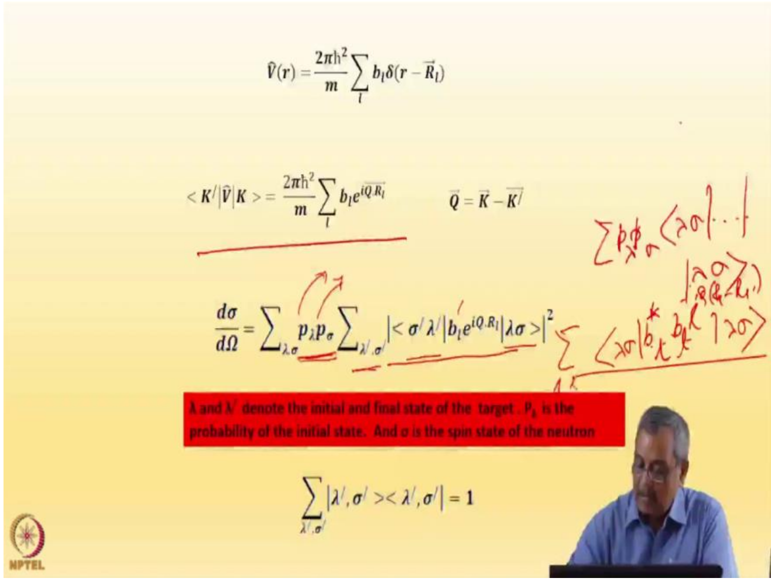


Now interestingly, I have a summation over, $\sum_{\lambda'\sigma'}|\lambda'\sigma' >< \lambda'\sigma'|$,what does it signify? This is in quantum mechanics known as a projection operator, you might have known it, but still, I will quickly explain to what it means.

It means that these are the all-possible final states. So, it is like a projection of the wave function into all the components in this space- $\lambda\sigma$ space. That means, for example, suppose I take a wave function ψ, if I can break it up into a basis vector, then ψ is nothing but = $\sum a_i\psi_i$ where ψ_i forms a basis vector set. And the fact is that just like normal classical geometry, if you add up three components of a vector, then the respective components, if I call them $\{a_i\}$, then their sum over a_i^2 should be equal to 1 because this is one component, this is this is another component and this is another component and if you see that the components are cosθ plus sinθ sinϕ plus sinθ cosϕ, if you add square of all these components, you will get equal to 1. This is exactly same only it may not be three dimensional, it can be higher dimensional, but the components will add up to one for the wave function.

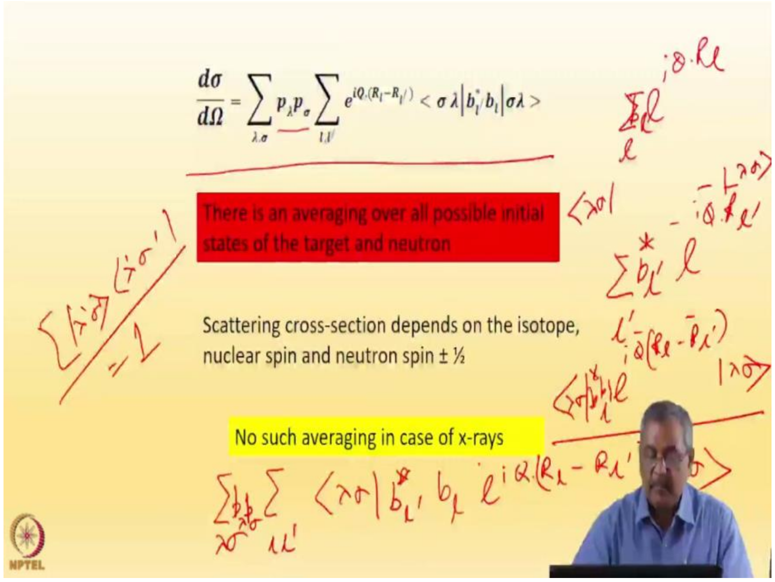
Here, if I pre-multiply and post-multiply with a wave function, then this is nothing but the component of this wave function projected on this, component of this wave function projected on this. So, I can call it a_i or I might call it $a_{\lambda\sigma}$ and these two multiplications gives me $a_{\lambda\sigma}^2$ and that is equal to 1. That's why in normal quantum mechanical parallels, I call this sum of the projection operators equal to 1.

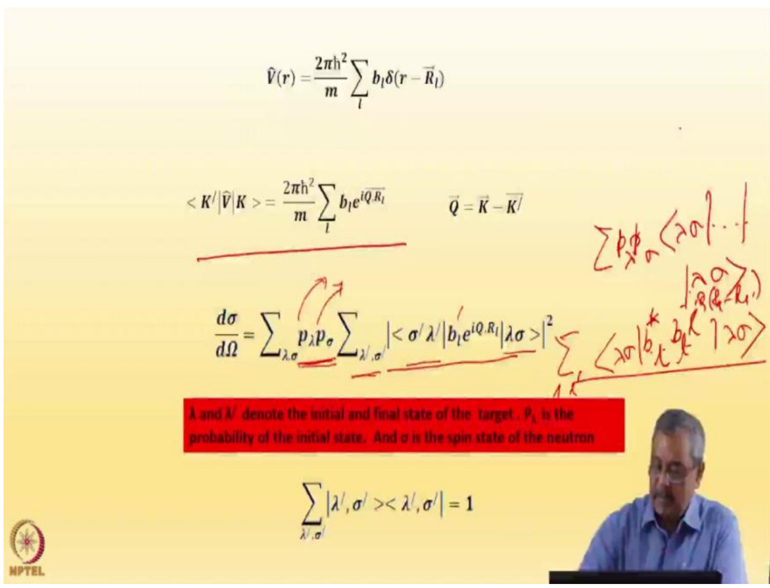
(Refer Slide Time: 07:55)



So, how does it help me here? Because of that, I can take the sum over all the final states. And then I can put them equal to 1 and then what I am left with sum over $p_\lambda p_\sigma$, λσ then the two complex conjugates of each other. So, I need to add up over all the initial states with this bracket notation λσ and then in between *l, l'*. I will have $\sum_{ll'} b_l b_{l'} e^{iQ.(R_l - R_{l'})}$.

(Refer Slide Time: 08:55)

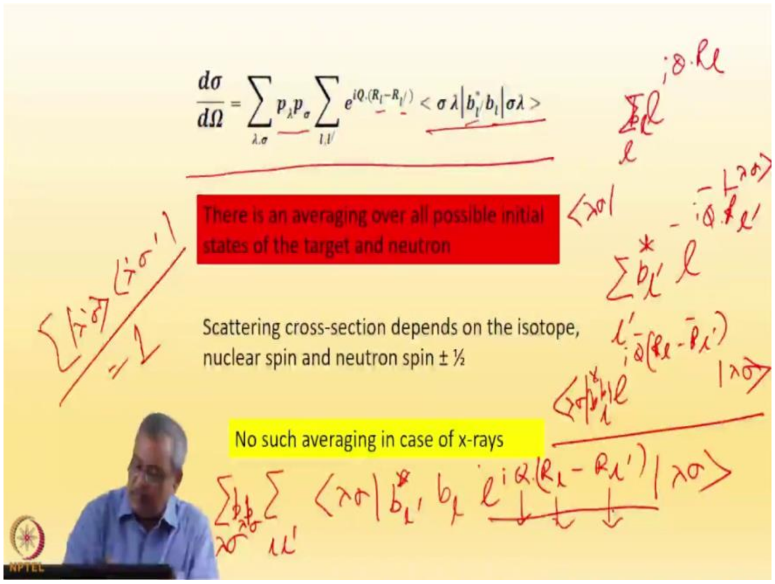




Stay with me, I will explain it once again. So, I had sum over *l* into $e^{iQ.R_l}$dl. When I do this summation, I also do this squaring. What I need to do actually, that I justified. But what more I have got is actually the complex conjugate of this is. ll' is a dummy variable, and another summation will be on l' $\sum_{l'} b_{l'}^* e^{-iQ.R_{l'}}$

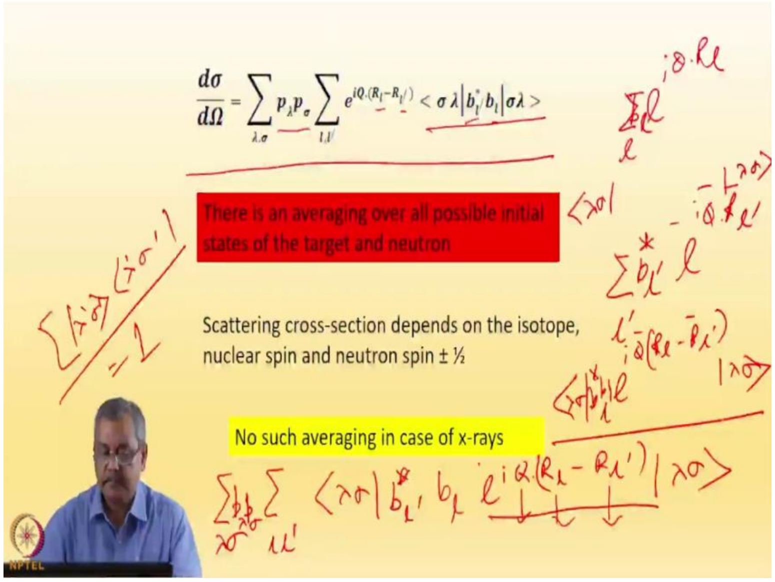
When I add these two in the middle of λσ what I get is $e^{iQ.(R_l - R_{l'})}$ then I have summation over λσ and I also have I have $\sum b_{l'}^* b_l$ in the pre factor. So, what I have got is $< \lambda\sigma | \sum_{ll'} b_{l'}^* b_l e^{-iQ.(R_l - R_{l'})} | \lambda\sigma >$. I have to sum up over all the sites, I have to sum up over all the initial states of spin- energy -isotope and of course, I have to take probability of the initial states. So, I have got $p_\lambda p_\sigma$ and I explained to you why the summation over $\lambda`\sigma`$ $\lambda'\sigma'$ was removed as they are sums over projection operator. I get $\frac{d\sigma}{d\Omega}$ equal to this expression.

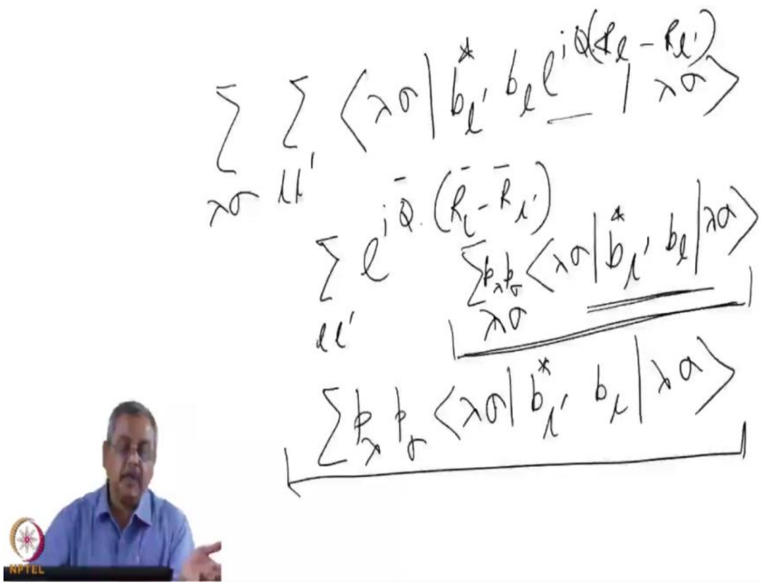
(Refer Slide Time: 11:07)



I hope I have been able to bring it home that this is the differential scattering cross section per unit solid angle given that the atoms (let me call them atoms or whatever) units that are sitting at the sites of corresponding scattering length b_l and $b_{l`}$ and I have to do the summation over all the initial states. Now, the question is I have written it like this over here, but you please see this expression cannot have any spin and isotope dependence because this is the wave vector transfer and I can take them outside.

(Refer Slide Time: 11:50)

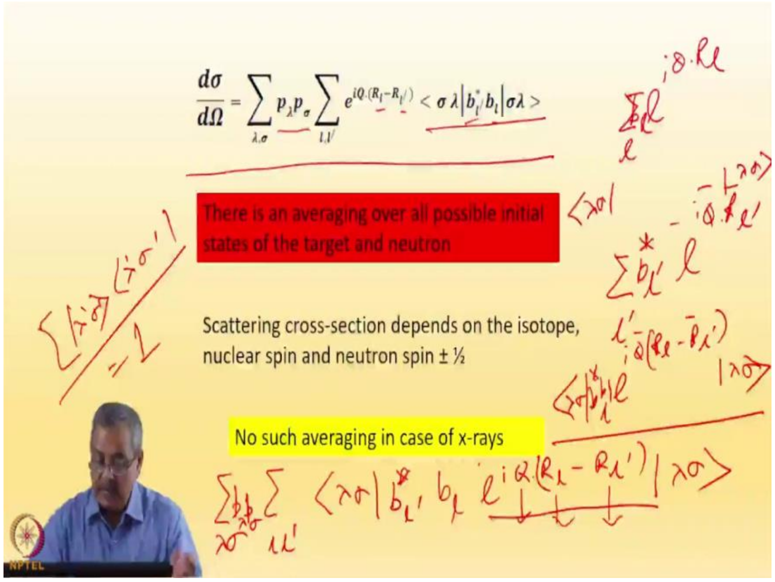


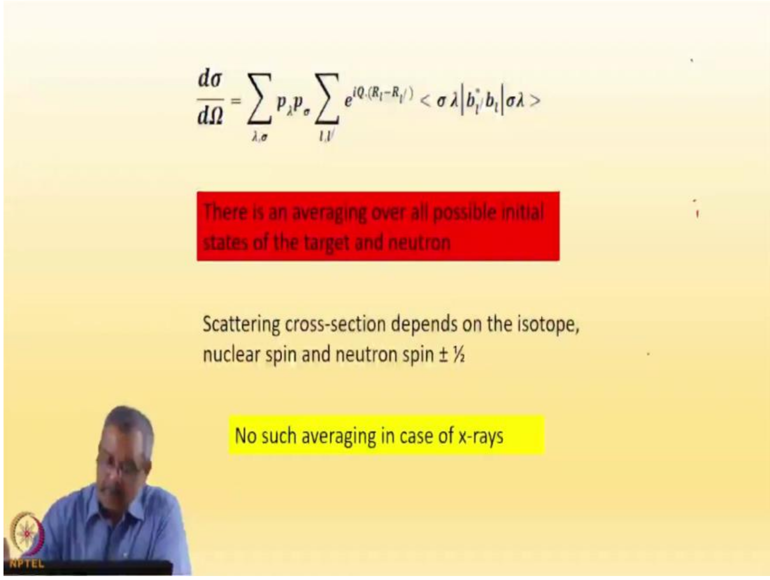


After taking them outside I have a summation over ll'. Earlier I had a summation over $\lambda\sigma$, now I have got $<\lambda\sigma| b_{l'}^* b_l e^{iQ.(R_l - R_{l'})}| \lambda\sigma>$. So, this exponential part does not have any dependence on isotope or spin. I can it take out of the summation. It means, now I have got sum over ll', $e^{iQ.(R_l - R_{l'})}$, but now, I have got $<\lambda\sigma| b_{l'}^* b_l| \lambda\sigma>$, that means this site at l' and l. There are scattering lengths which depend on the isotope, energy etc. if you talk about energy changing. It also depends on the spin of nucleus versus the neutron spin, up or down.

And this averaging (sorry again I missed here the sum over $p_\lambda p_\sigma$) with respect to the initial probabilities. It is something which is unique for neutrons, because the scattering length is dependent on isotope and spins, varying from site to site and in this averaging we need to do so. It means, we need to find out this part, which we will deal later. $p_\lambda p_\sigma$,This is an averaging over the entire sample, which we have to perform.

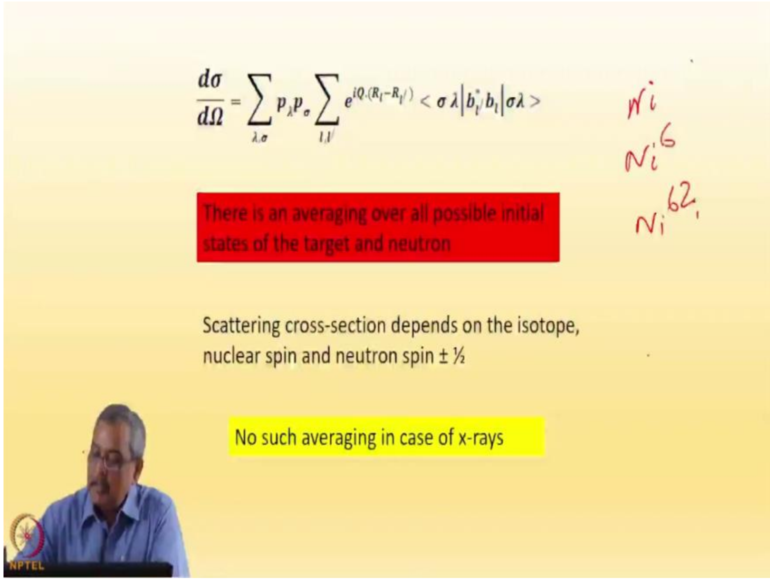
(Refer Slide Time: 14:17)

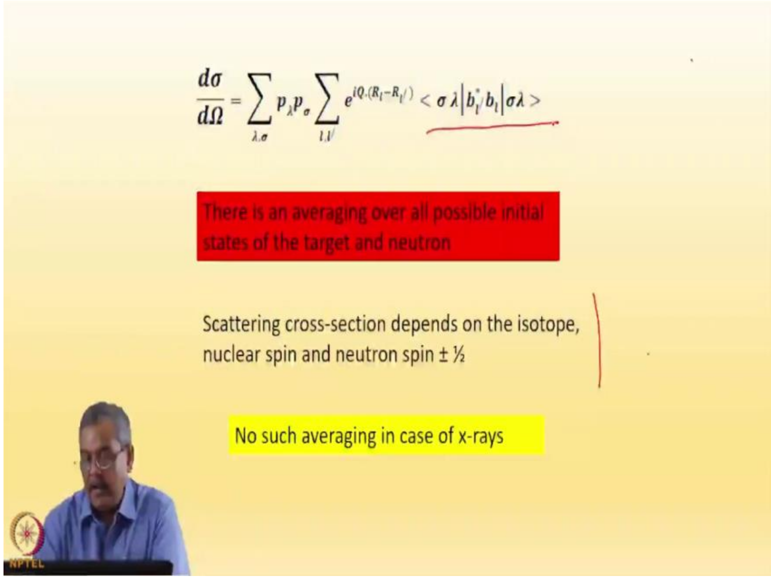




Please look at this expression. This is what I was trying to reach through this discussion. Now, this is unique about neutrons and this you will not see for x-rays, which is the closest cousin of neutrons so far as diffraction is concerned and why not? I will explain to you in my talks later and also today. Because, in case of x-rays, the scattering is from the charge cloud around a scattering particle like an atom and this charge cloud does not vary from site to site. It does not depend on let say polarization of x-rays or it also does not depend on the isotope.

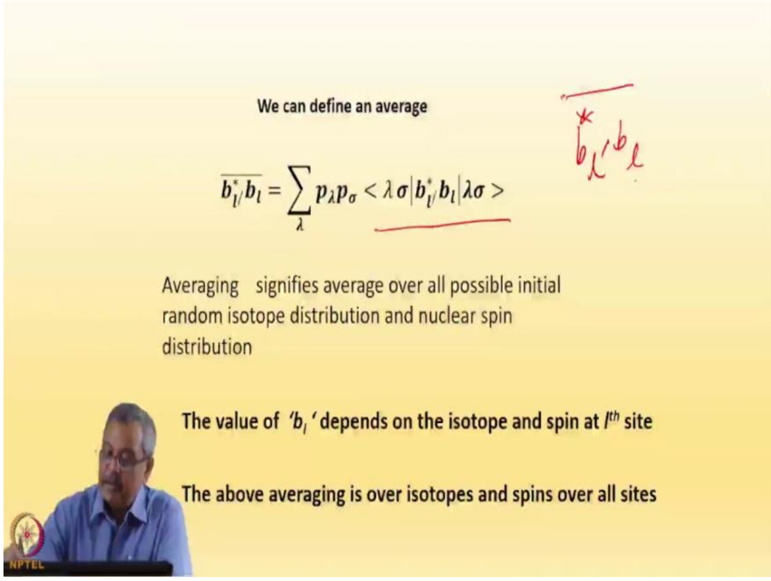
(Refer Slide Time: 15:18)

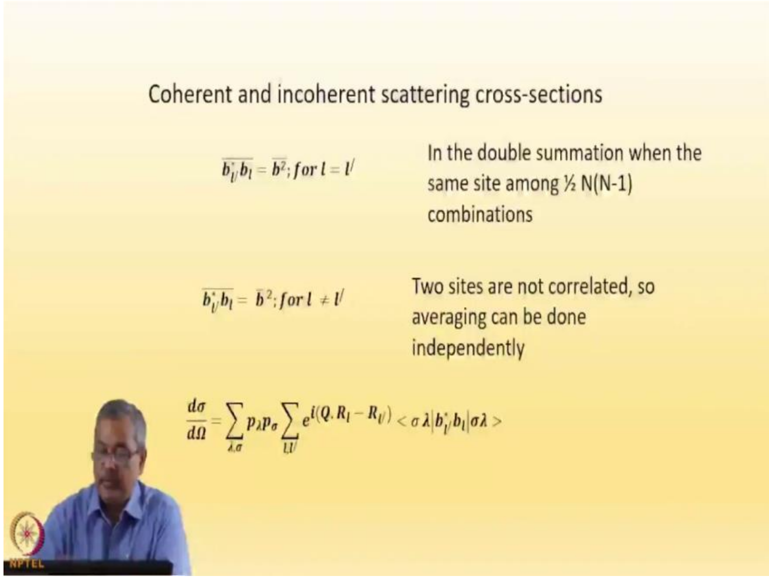




I mean, if I am talking about scattering from nickel, then, Ni and Ni^{62} are two isotopes. Their charged cloud size is the same and so, there is no variation, so, far as x-ray scattering length is concerned. But, scattering cross section depends on the isotopic nuclear spin and neutron spin and that is contained in this summation.

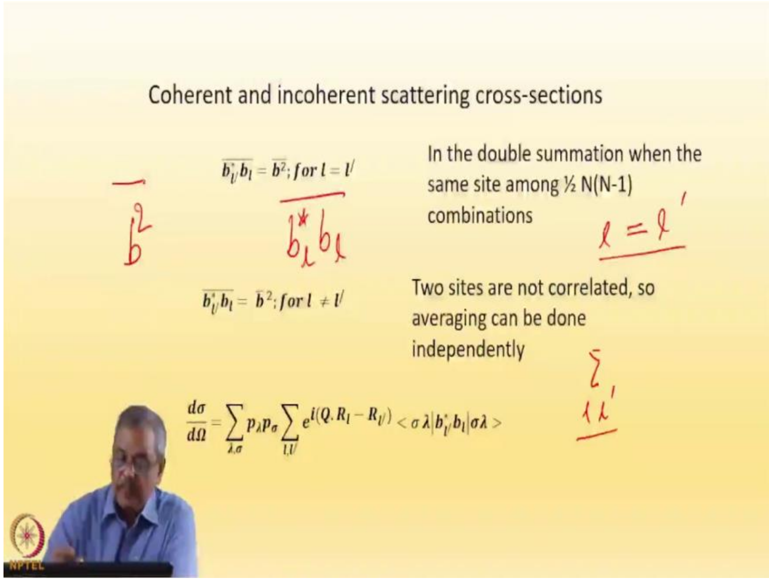
(Refer Slide Time: 15:41)

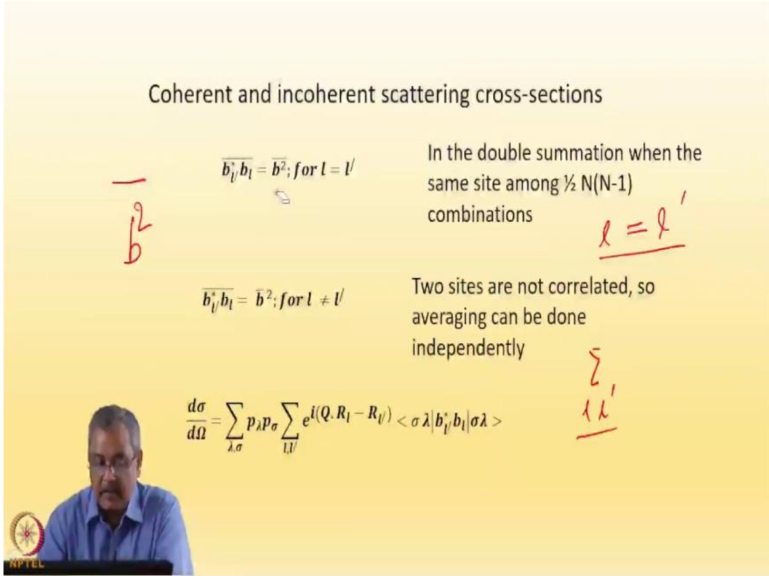




Let me say we need to now define an averaging process in which the summation is over ll'. I need to do an averaging over initial states. So, this is an average value of $b_l b_{l'}$ and summation over that.

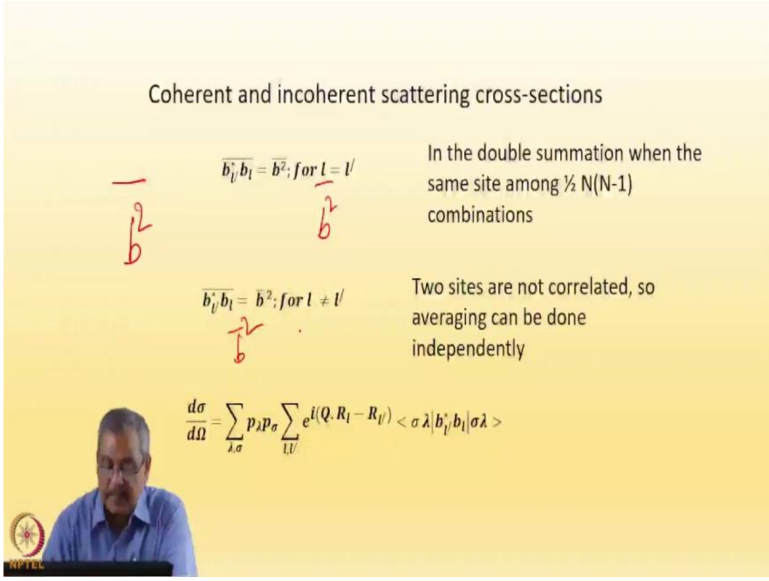
(Refer Slide Time: 16:09)





There are two parts to it. Let me come to what I call as coherent and incoherent scattering cross section. In this double summation, which is a summation over *ll'*. Now, you imagine, I am talking about a lth site and an l' site. There are (1/2)N(N-1) pairs now; in that count, when I am talking of the same site that is $l = l'$ then it is $b_{l'}^* b_l$ and an average over that and that is nothing but b^2 and average of that. So, that means for $l = l'$ it is b^2 average.

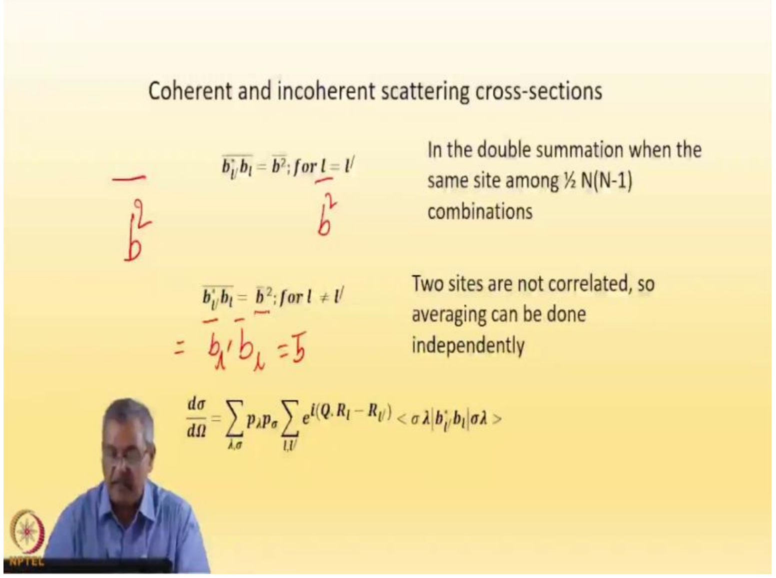
(Refer Slide Time: 17:08)



But when $l \neq l`$, let us assume that the isotope and spin in one site has no correlation with the isotope and spin at the other site except for that they are statistically correlated, it means that if an isotope has 1% abundance, then a site will have that particular isotope as a probability of 0.01 and other isotopes will be 99.99. So, if it is a 10% abundance, then the probability the site will have that isotope is 0.1 or the probability will not have the isotope there is 0.9.

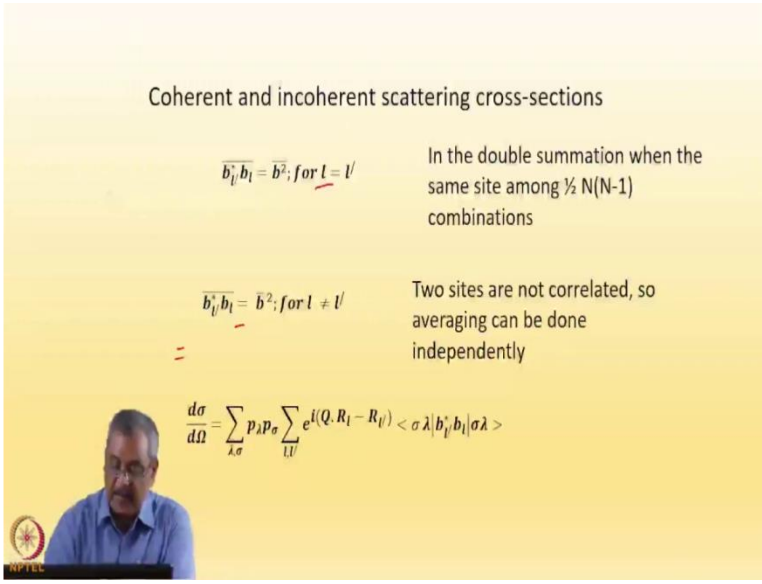
It is only statistical averaging. So, then $b_{l`}^{*}b_l$ average will be given by, for l ≠ l`, only b average over isotopes, and then square of that, so, I have got one b square average (l = l`) and when l ≠ l`, because they are not correlated, I will do the averaging separately.

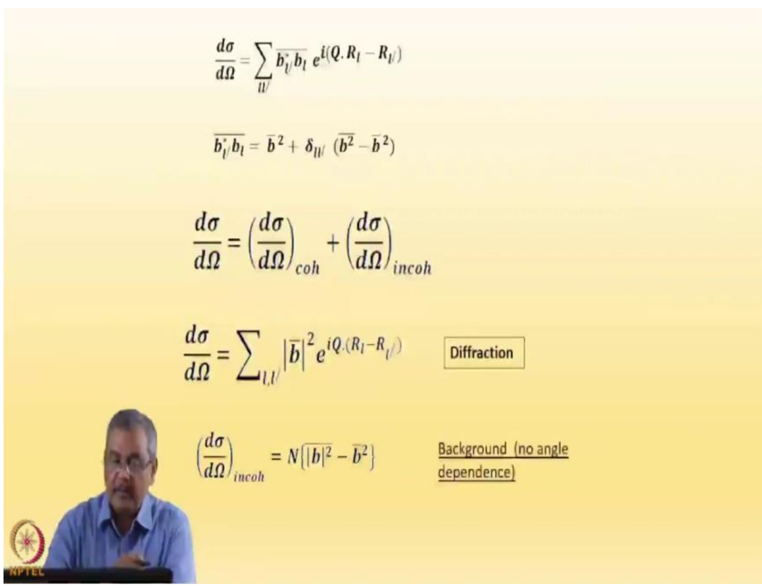
(Refer Slide Time: 18:17)

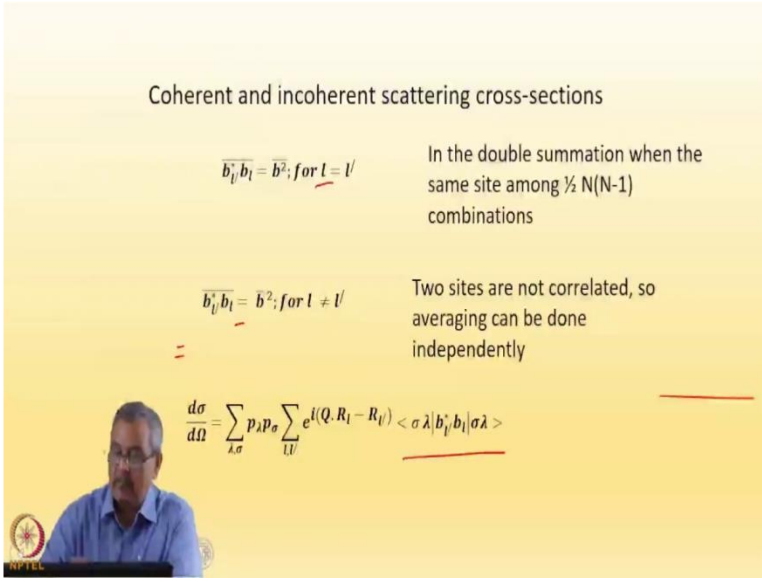


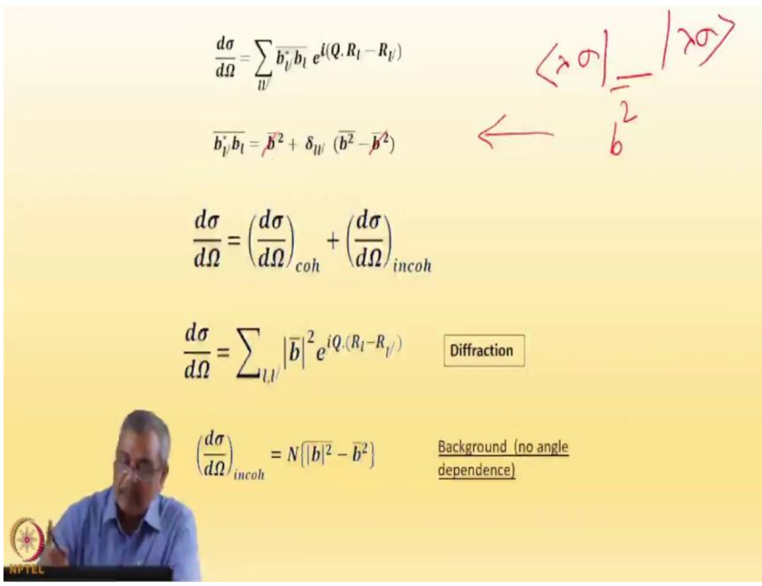
So, let me just write one more line, this is equal to $< b_l >$and $< b_{l'} >$. Now, there is nothing to choose between two sites and these two averages must be same. If I do over the entire sample the summation, these two averages should be same, and they should be b average, and this will give me b average square. So, I have got a b square average and I have got a b average square.

(Refer Slide Time: 18:48)







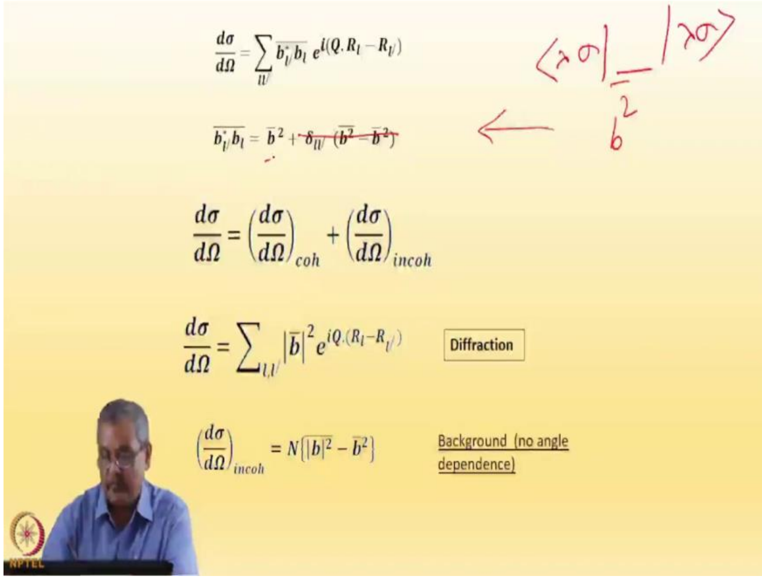


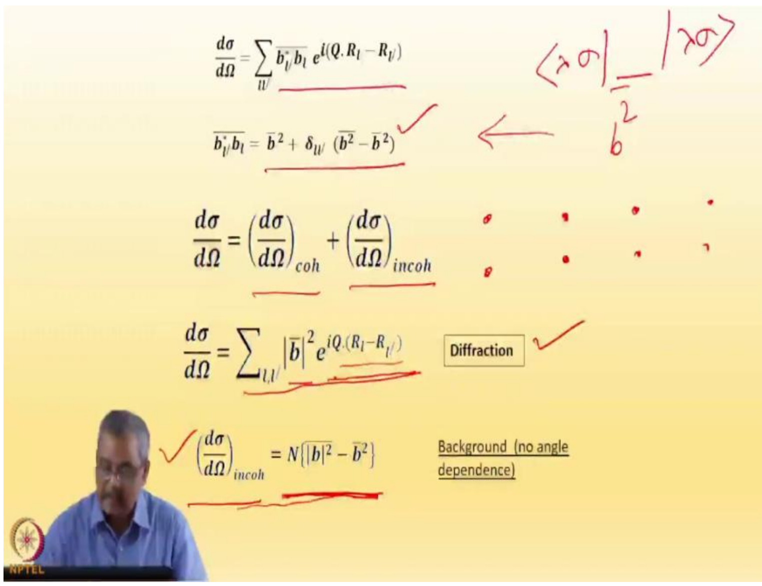
Now, please note that $\frac{d\sigma}{d\Omega}$ I have to do this averaging what I get is this one, summation over ll'. We know this averaging is over λσ. Please note that, this summation I have not done yet. The averaging is only over λσ.

In this average when l = l' then it gives me $< \overline{b^2} >$ and when l ≠ l' then it gives me $< \bar{b}^2 >$.

Look at this expression when $l = l'$wrote it as equal to $< \bar{b}^2 >$ and when $l \neq l'$ $\sum_{ll'} \delta_{ll'} [< \overline{b^2} > - < \bar{b}^2 >]$. So, when l = l`, then these two will cancel out.

(Refer Slide Time: 20:14)



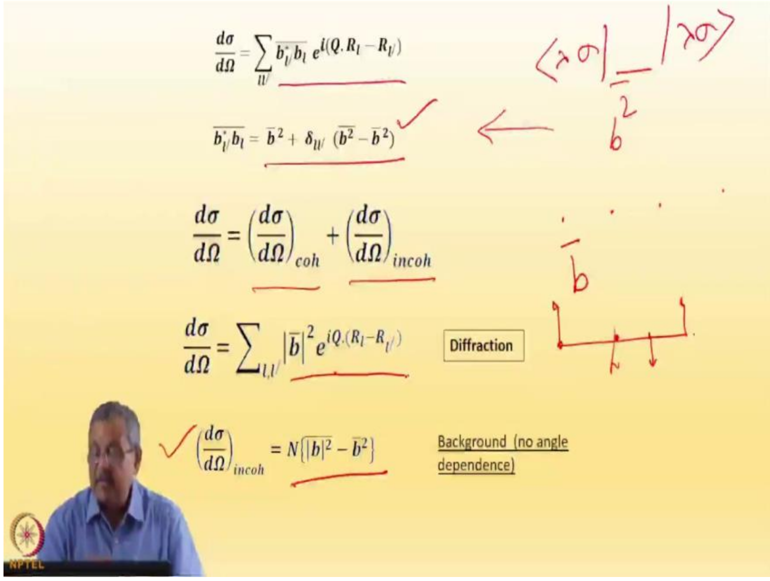


And when $l \neq l`$, then then this term is 0, I have b average square, which is what I said that when $l \neq l`$, you have got a b average squared, because two sites are independent of each other and averaging is being done over isotope and spin. So, it will be b average and square of that.

But now, with this expression, I can write $\frac{d\sigma}{d\Omega}$ into two parts, one is coherent part and other one is incoherent part. You please note that $\frac{d\sigma}{d\Omega}$ I am defining as b average square $e^{iQ.(R_l - R_{l`})}$ sum over ll`, that is when $l \neq l`$.

This expression gives me $iQ.(R_l - R_{l`})$ for a lattice, this is the expression which gives me diffraction. And look at the other expression because when $l = l'$, then $e^{iQ.(R_l - R_{l`})}$ goes to 1 and I have got this summation gives me (summation over ll`), because $l \neq l`$ will not be there. N into this is what I wrote b square average minus b average square and see this has no dependence on a $Q.(R_l - R_{l`})$. It has no angular dependence. This is that is why I call it incoherent because (it has no angle dependence and this expression has got angle dependence, which gives me diffraction) this does not have any angle dependence and this will give me a background.

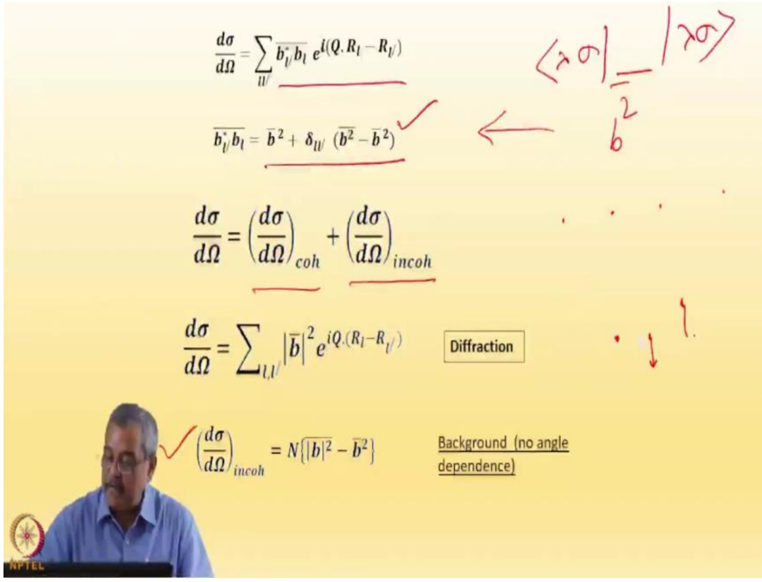
(Refer Slide Time: 22:30)

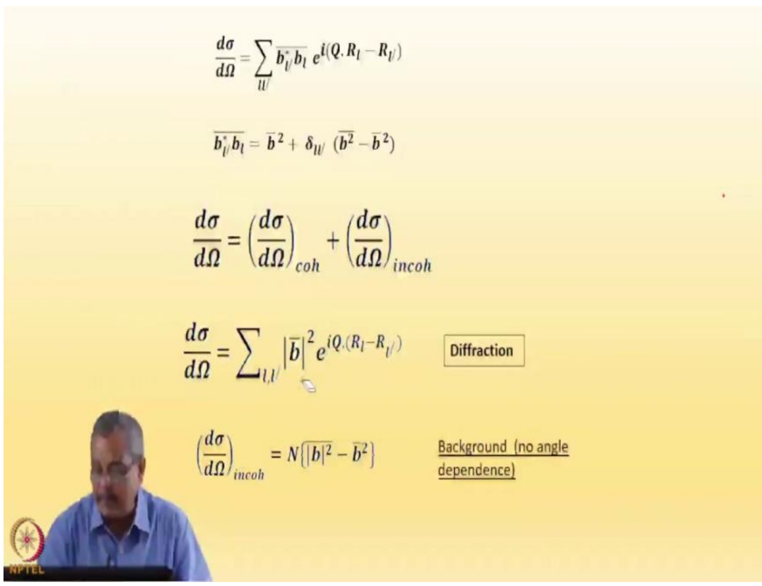


So, in case of neutron diffraction, b square average minus b average square term gives me incoherent scattering. Incoherent means, the scattering from one site is not correlated with the scattering from another site and it gives me a background and when I talk about coherence, then I talk about b average.

Basically, when I go from site to site, there is a mean scattering length, when I go from one site to another site to another site to another site. When I do the averaging over all the spins and initial states, I have got a b average sitting at every site and also there is a fluctuation, so there is a mean value and there are fluctuations around this, and this fluctuation is an incoherent background. The expression with the b average gives me diffraction.

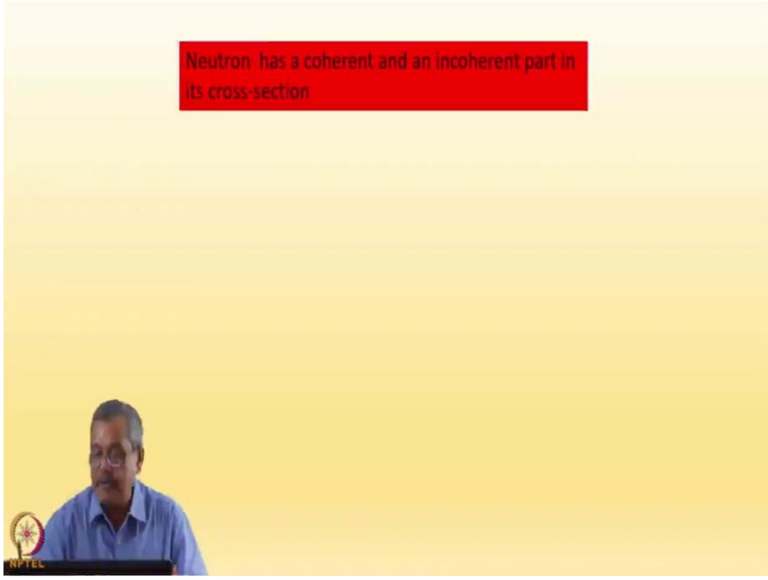
(Refer Slide Time: 23:18)

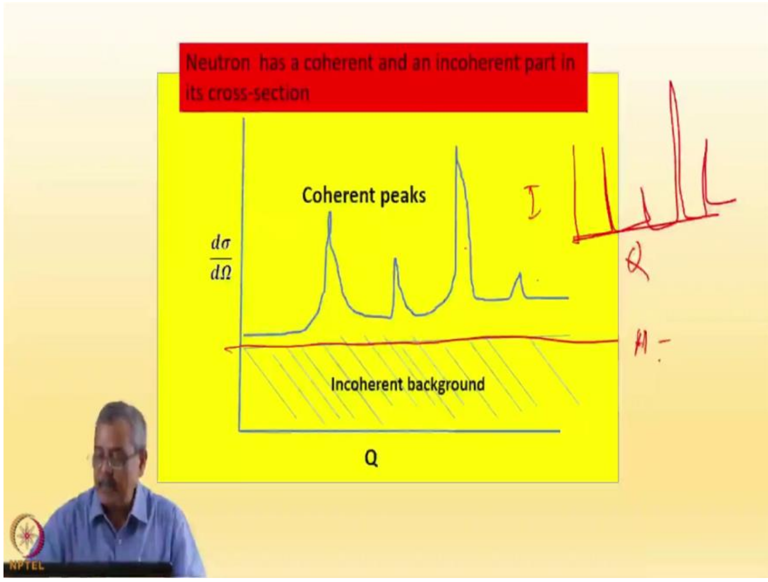




This is completely different from what you find in x-rays, because in x-rays, the charge cloud does not change from site to site. So, there is nothing like b square average minus b average square for x-rays. I will explain to you later and derive for you that b average is comparable to form factor for x-rays. If you are familiar with x-ray diffraction, you know what is the form factor.

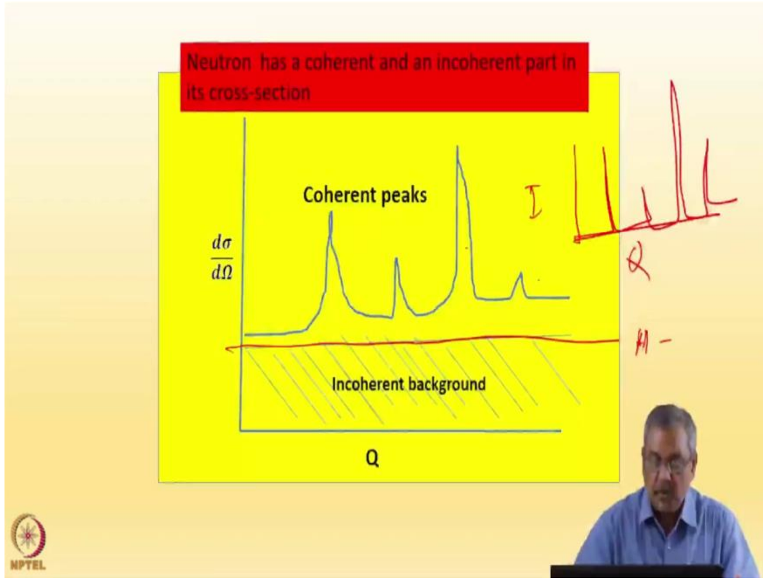
(Refer Slide Time: 23:53)

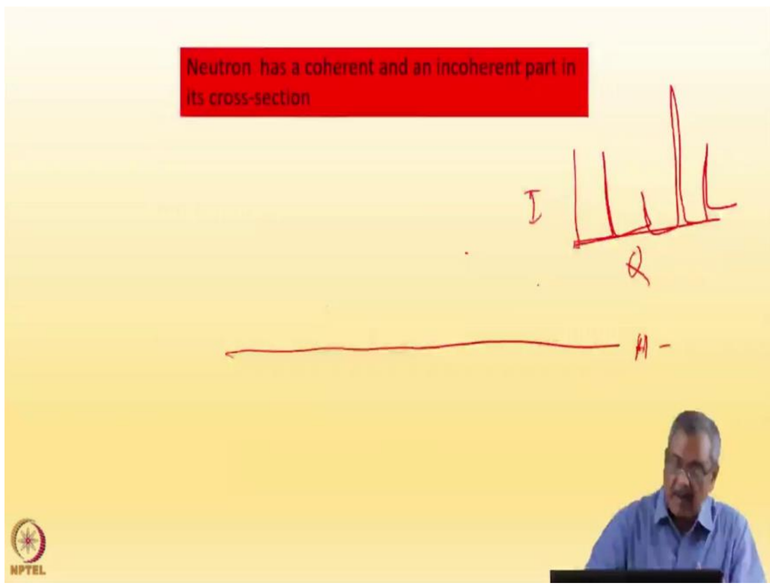




So, now, neutron has a coherent and incoherent part in its cross section, and it will have lots of implications which we will discuss later. Excuse my bad drawing, what you find as intensity versus Q in case of neutron diffraction you get Bragg peaks, this is what I mean comes from b average, these coherent peaks and also we have an incoherent background line below it, if you have incoherent scattering cross section non zero for that particular sample. For example, one of them is hydrogen, which has got a very large incoherent cross section and why I will explain to you later.

(Refer Slide Time: 24:31)


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


Neutron has a coherent and an incoherent part in its cross-section
I
Q
H -
NPTEL

$$\frac{d\sigma}{d\Omega} = \sum_{ll'} \overline{b_{l'}^{*} b_l}\, e^{i(Q.R_l - R_{l'})}$$

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

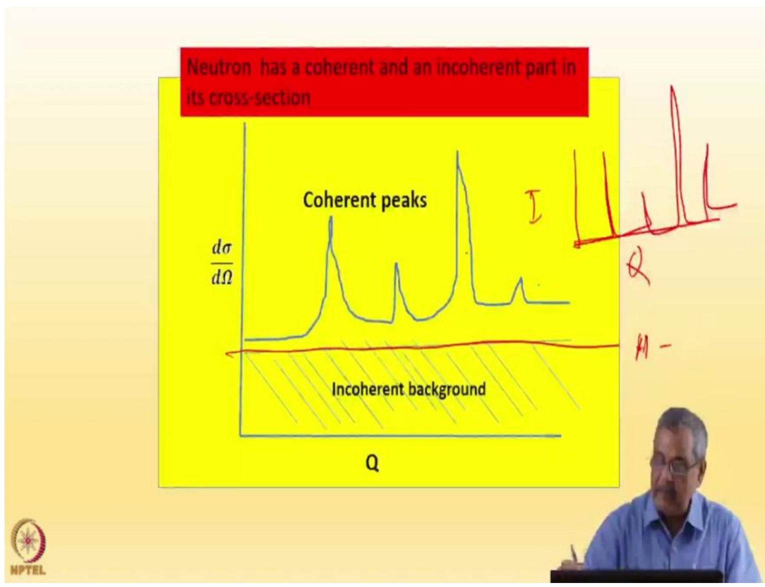
$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_{coh} + \left(\frac{d\sigma}{d\Omega}\right)_{incoh}$$

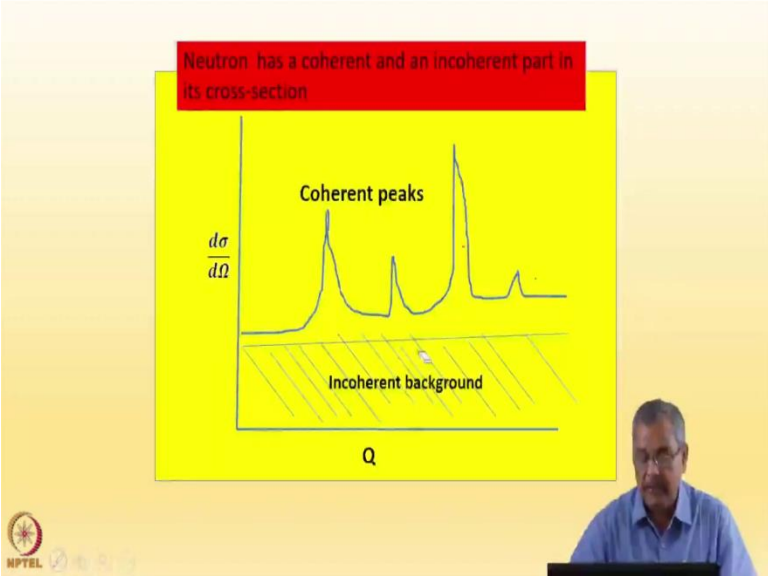
$$\frac{d\sigma}{d\Omega} = \sum_{l,l'} |\bar{b}|^2 e^{iQ.(R_l - R_{l'})}$$

Diffraction

$$\left(\frac{d\sigma}{d\Omega}\right)_{incoh} = N\{|b|^2 - \bar{b}^2\}$$

Background (no angle dependence)





So, now, let me consolidate. I had started with Fermi golden rule, I derived scattering amplitude, then I derived the scattering cross section, $\frac{d\sigma}{d\Omega}$ the angle dependent scattering cross section. Then I did an averaging over the initial states of spin and isotope and I showed you that we have a coherent part which gives me diffraction and an incoherent part which gives you background and this is unique about neutrons. With this I come to the end of this lecture. More discussions will follow regarding neutron diffraction in the later lectures. Thank you.