Neutron Scattering for Condensed Matter Studies
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Week 02
Lecture 05 B

Keywords: Fermi pseudo potential, Diffraction, Scattering law, Debye-Waller factor, Ensemble average, Coherent Scattering, Incoherent Scattering

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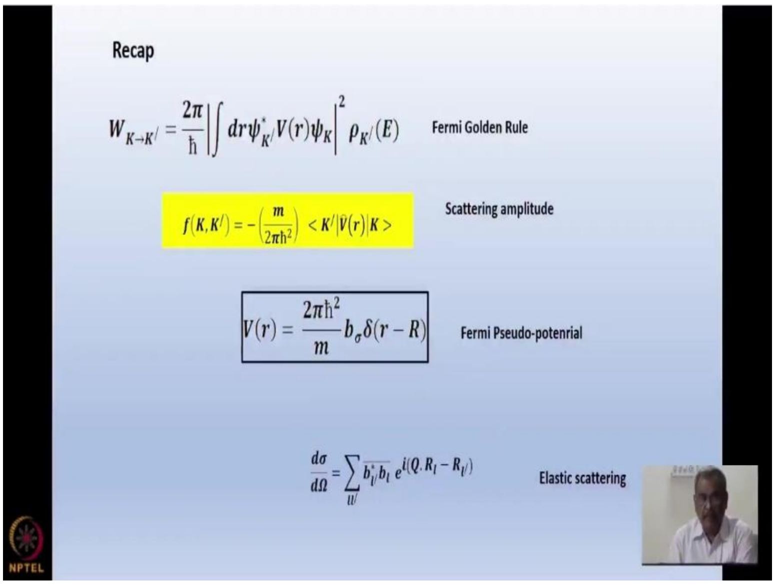

Before I go further, I just want to quickly recap what we have done so far in the previous four lectures. I started with Fermi golden rule where I narrated that the starting wave function with vector K (ψ(K)) goes to ψ(K′) under the influence of potential V(r), in general, in a scattering system. There is also a term, density of states $\rho_{K'}$(E) which is required as we are talking about the transition from one state to another.

From there, I went ahead and derived the scattering amplitude f(K, K′), which is $-\left(\frac{m}{2\pi\hbar^2}\right)\langle K'|\hat{V}(r)|K\rangle$. It is in the bracket notation where $|K >K$ is for $e^{iK.r}$ and $< K'|\ K'$ is for $e^{-iK'.r}$ along with some constant and it is an integration over 'r' for both of them.

I assumed a delta function potential known as Fermi-Pseudo potential for the scattering system. I have assumed that only neutron and nucleus interaction is acting and because nucleus is very tiny (femto-meter) size compared to the wavelength of the neutron which is of the order of Å, hence I can assume it as a delta function potential. In the expression for this potential here, b_σ is a spin/isotope dependent scattering length for the site R where the delta function is sitting.

With these two, I found that the elastic scattering, here elastic means no energy transfer between the neutron and the scattering system, cross-section is given by,

$$\frac{d\sigma}{d\Omega} = \sum_{ll'} \overline{b_{l'}^{*} b_l}\, e^{iQ.(R_l - R_{l'})} = |f(K, K')|^2$$

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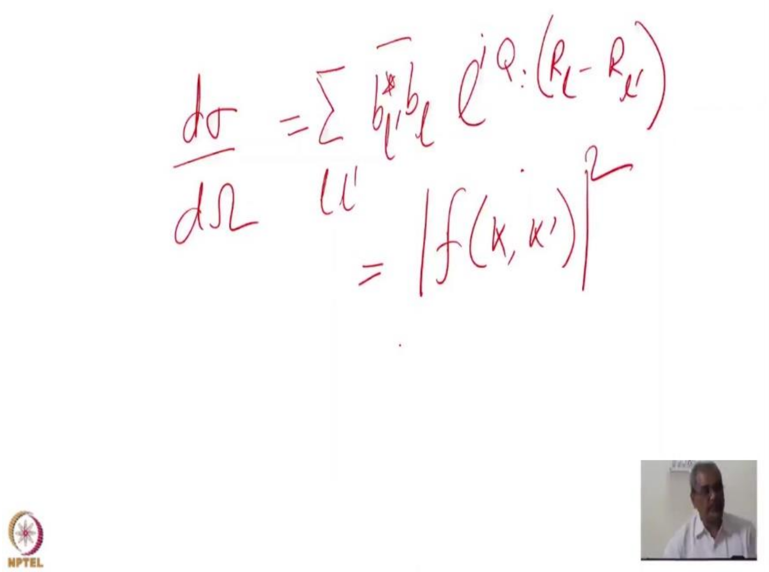

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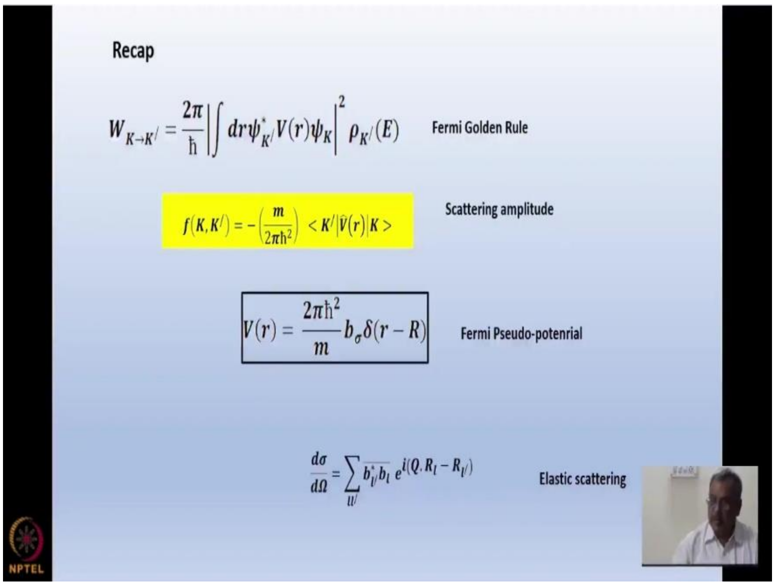

This is elastic scattering cross-section.

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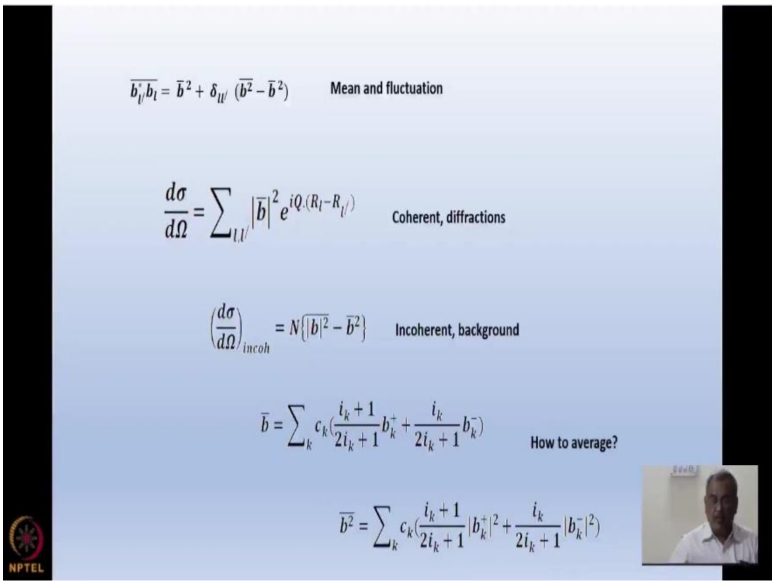

While calculating the elastic scattering cross-section, we have to evaluate $\overline{b_{l'}^{*}b_l}$, where averaging is over all the isotopes, spins in the lattice. This term has two parts. One of them is b average square ($\bar{b}^2$) where b average is the mean potential seen by the neutron when you average over spin and isotope of the scattering system. And the fluctuation around the mean which is given by $\delta_{ll'}$ ($\overline{b^2} - \bar{b}^2$). When I write down the scattering cross section in terms of these two, I get two parts. One is the coherent part, $\sum_{ll'} \overline{b_{l'}^{*}b_l}\, e^{iQ.(R_l - R_l')}$, which causes diffraction. As we have $Q.(R_l - R_l')$ term here, so, we need to know the position of the l' with respect to position of the l and in a crystallography lattice these are fixed. Whenever diffraction occurs then we know that Q will be equal to reciprocal lattice vector G and $R_l - R_l'$ will be given by the miller indices.

Another part is $N\{\overline{b^2} - \bar{b}^2\}$. This is incoherent part and unlike coherent part it has no angle dependence.

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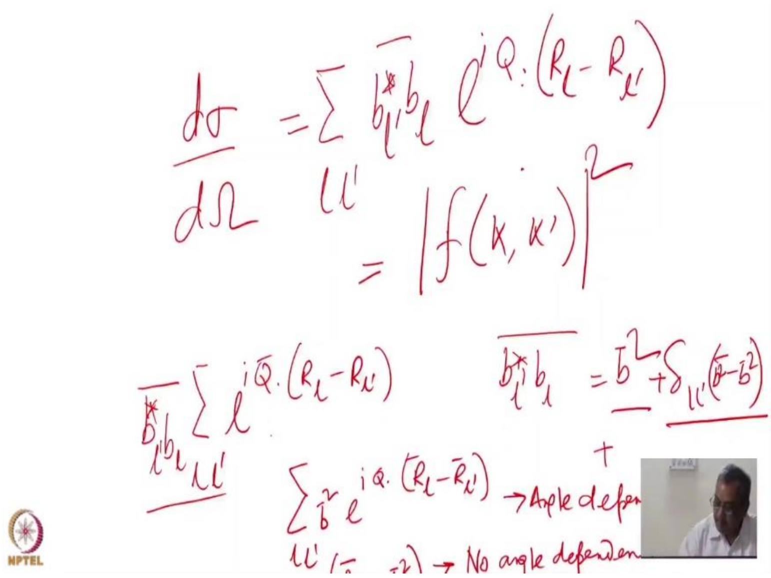

Hence, we can write $\overline{b_{l'}^{*}b_l}$ as $\bar{b}^2 + \delta_{ll'}\left(\overline{b^2} - \bar{b}^2\right)$, where 2nd term is the incoherent part and 1st term is the coherent part.

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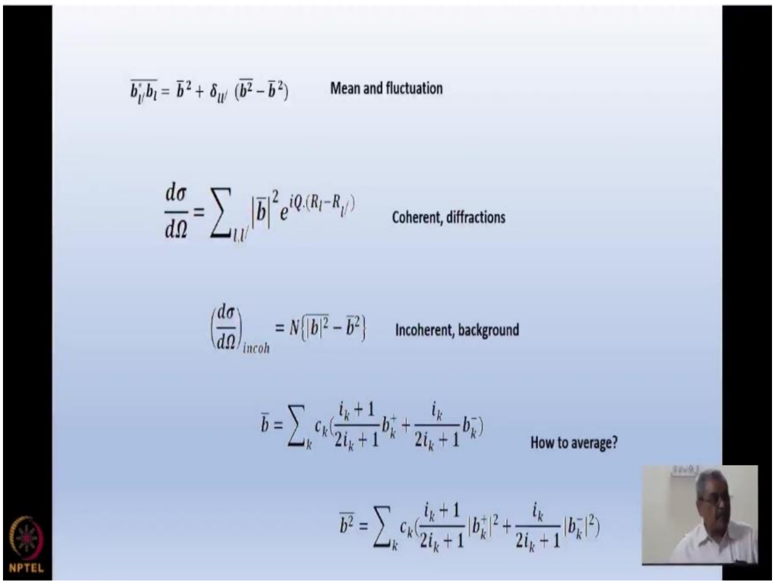

I also showed you how to find out $\bar{b}$ for a distribution of isotopes and spins if I have a k^{th} isotope having nuclear spin i_k then $\bar{b}$ is given by the relative statistical weight of the two states with the neutron spin is parallel and anti-parallel to the nuclear state.

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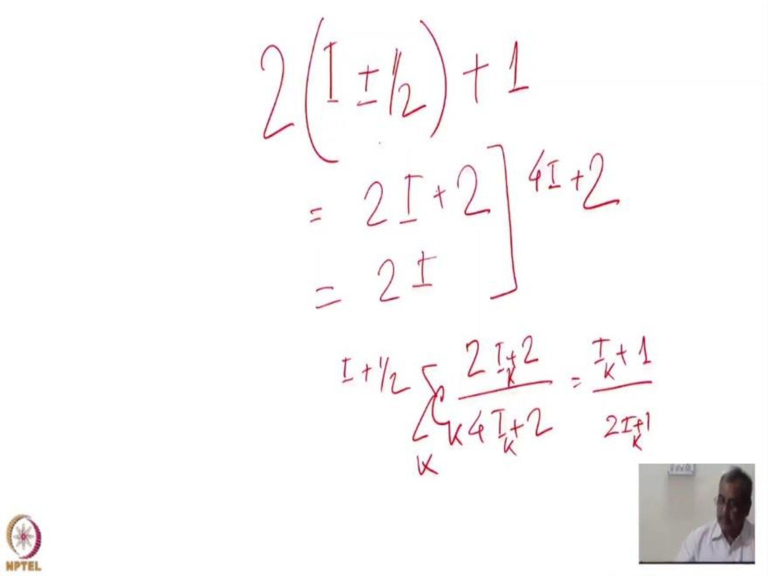

If the nuclear spin is I and the neutrons spin can be ±1/2 then the number of states will be 2(I±1/2) +1. For +1/2, it will be 2I+2 and for -1/2 it will be 2I. Adding these two, the total weight becomes 4I+2. In this way, the relative weight for I+1/2 states is (I+1)/(2I+1) and for k^{th} isotope it will become (I_k+1)/(2I_k+1) and then we will have isotopic summation over concentration of k^{th} isotope multiplied by this factor. It goes like this.

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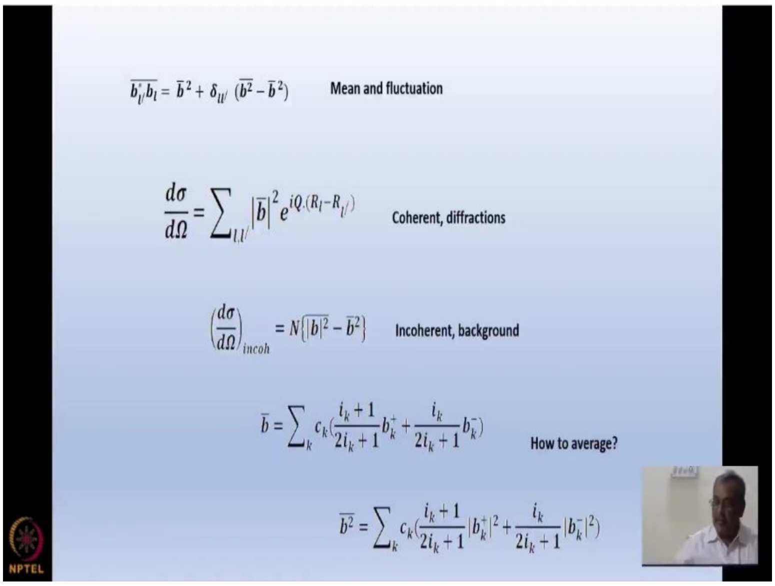

Hence, average scattering length $\bar{b}$ can be written as,

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

where c_k is the concentration of the k^{th} isotope, b_k^+ is a scattering length for the neutron spin in direction of the nuclear spin and b_k^- when the neutron spin is in opposite direction to the nuclear spin. b_k^+ and b_k^- can be found experimentally. Similar to this $\overline{b^2}$ is given by,

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

With these $\bar{b}$ and $\overline{b^2}$ we can find out the coherent and incoherent scattering cross sections.

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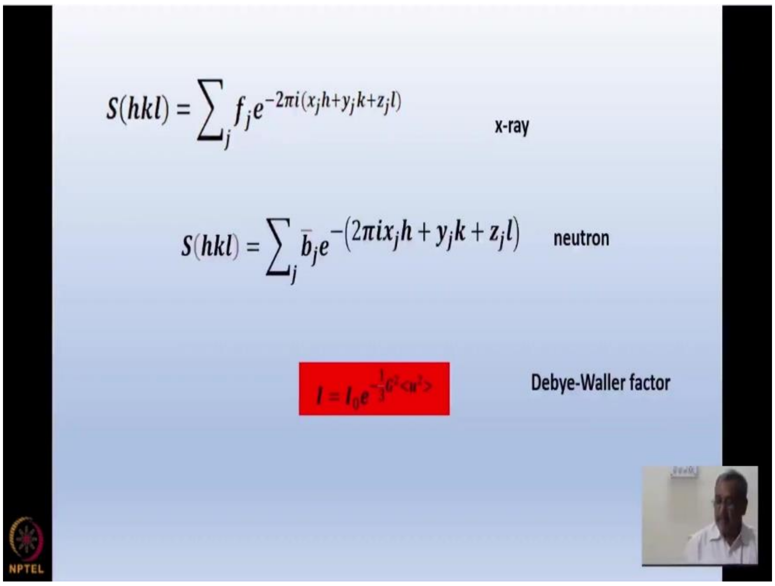

I also told you that the scattering amplitude S(hkl) for x-ray is given by

$$\sum_j f_j e^{-2\pi i(x_j h + y_j k + z_j l)}$$

for an *hkl* plane where the positions of the atoms are given by $ax_j + by_j + cz_j$. For neutron, f_j gets replaced by the average scattering amplitude b_j which is basically a delta function potential. f_j is a form factor which has got a Q dependence and the intensity in case of x-ray peaks go down at the higher angles. This is not the case for neutron because b_j does not have any angle dependence, it is constant all over Q space.

Afterwards, I introduced you to the Debye Waller factor for what happens when the atoms are at a finite temperature or the system is at a finite temperature *T*. They oscillate around the mean position. The amplitude of oscillation u^2 around the mean position tells us the intensity falls as, $I_0 e^{-\frac{1}{3}G^2\langle u^2 \rangle}$ where G is a reciprocal lattice vector at which we are measuring the intensity the

Bragg peak and I_0 is the 0 K intensity. Hence, with increase in temperature, as long as the lattice is there, which means mean position of the lattice is not destroyed, the vibration around the mean position causes a drop in intensity not disappearance of the Bragg Peak. Only when the lattice starts melting the Bragg peak disappears.

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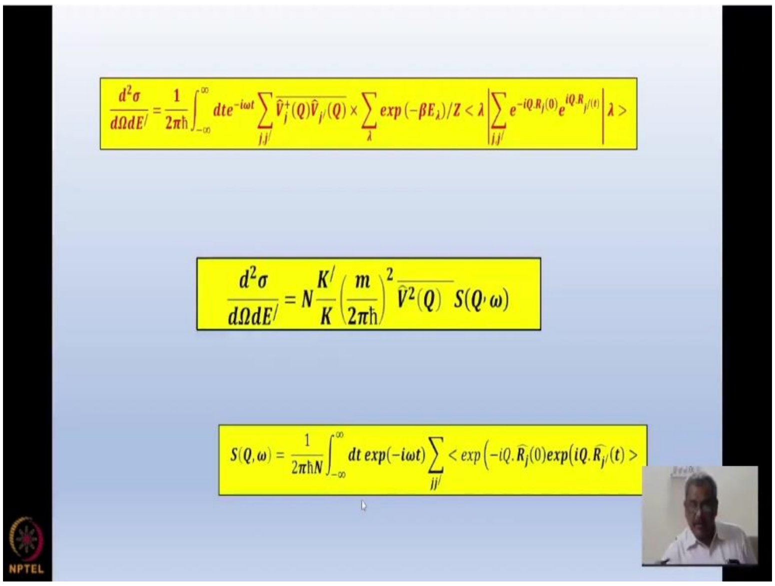

Following this, I brought in the time dependence through a delta function and this is what I wrote again and again. We have an average of the potential at j and j' summed over jj'. We also have Boltzmann's weight for every state and the statistical average of $e^{-iQ.R_j(0)}e^{-iQ.R_{j'}(t)}$ which is a correlation function and I also showed you that S(Q, ω) is a Fourier transform of this correlation function.

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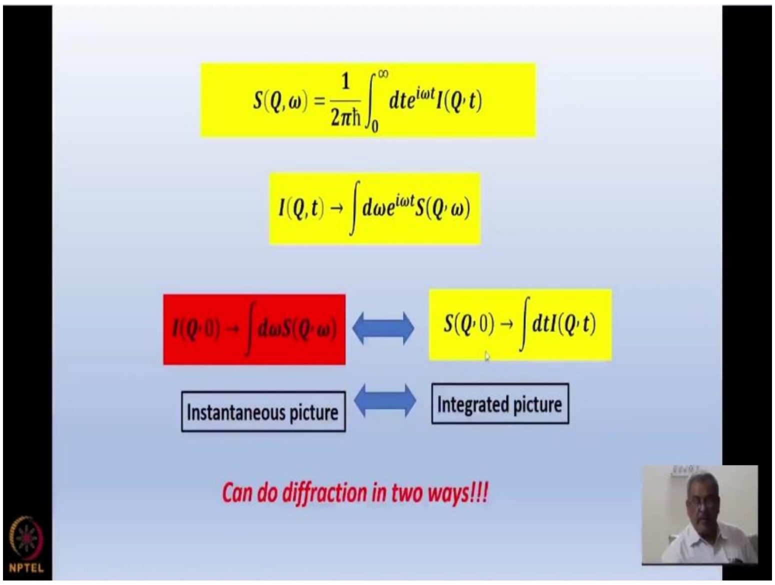

Then I showed you that $S(Q, \omega)$ is a Fourier transform of intermediate scattering law $I(Q,t)$ and $I(Q,t)$ is just the opposite way, is a Fourier transform $S(Q, \omega)$. We have

$$I(Q,\omega) \longrightarrow \int d\omega\, e^{i\omega t}\, S(Q,\omega)$$

In this expression, if I put t = 0 then $I(Q,0)$ is given $\int d\omega\, S(Q,\omega)$ that means, at any instant of time the intermediate scattering function is seen as an integration of $S(Q, \omega)$ over energy space. The other way round, if I put $\omega = 0$ that means, a process of scattering in which energy transfer is equal to 0 this $S(Q, 0)$ is $\int dt\, I(Q,t)$, that means when I look at diffraction with perfect 0 energy transfer that gives me an average picture over time.

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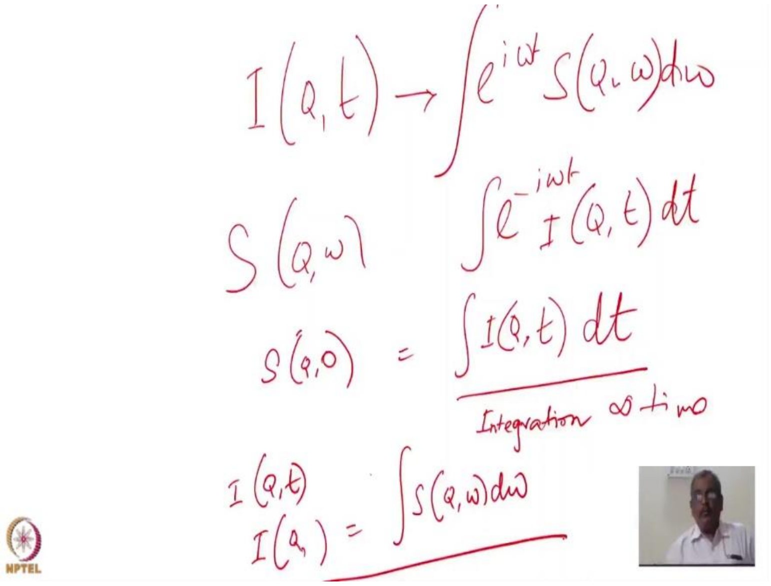

In this integration, you are looking at the system over infinite time whereas, if I consider *I*(Q,t) then any instant of time ‘*t*’, which I call origin of time, *I(Q)* is given by integration over all the energies. What does it mean? Let us see, how we do the diffraction experiment,

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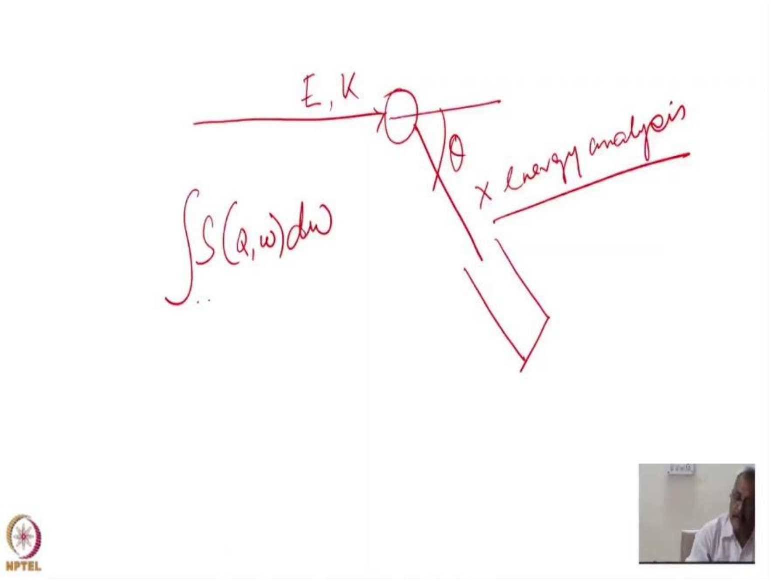

I have put an incident beam, a sample and then I have got a detector here. I will also tell you later how the detector works. I count the neutrons on the detector. Here, usually, I do not do any energy analysis, so, in this case, what I am doing is actually, integrating S(Q, ω) over ω. We are integrating over whatever energy is coming to the detector.

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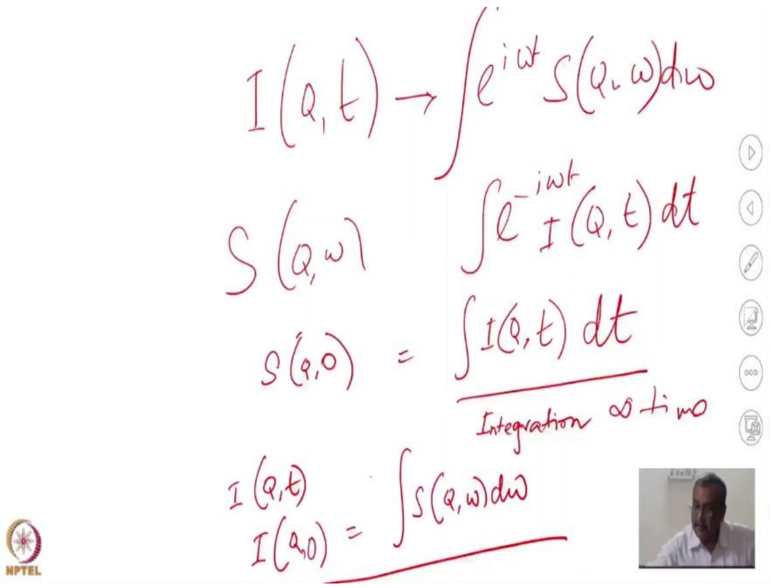

I told you just now that with this integration what I get is an instantaneous picture.

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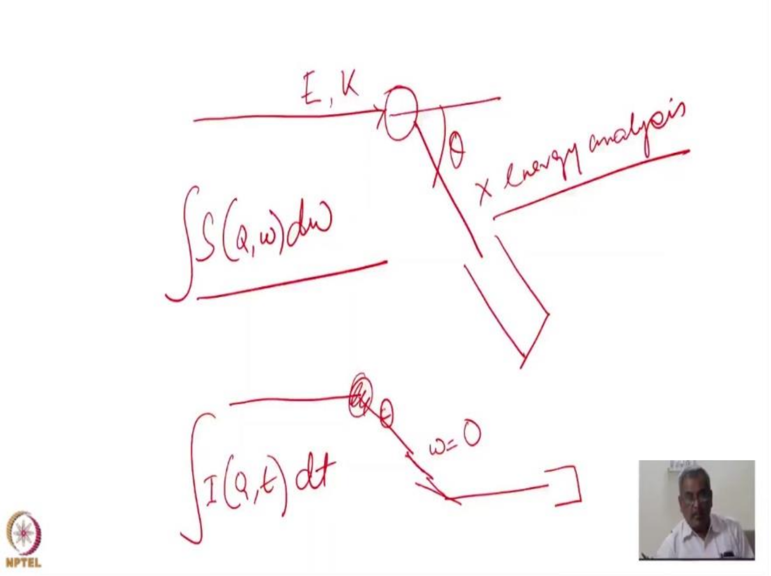

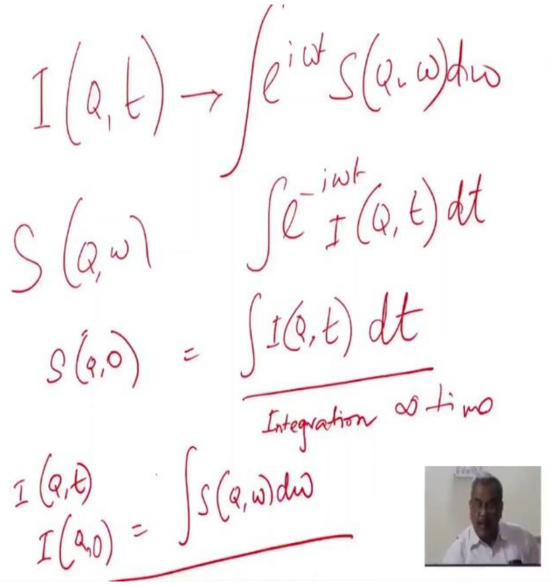

On the other hand, if I do an experiment with the same configuration, but, after the sample at an angle θ, I ensure that I measure only those neutrons which have got ω = 0. How do I do it? I can do it by putting another crystal to select the energy of the neutrons and then I can put the detector here.

If I do that, then what I have is actually integration over all the time. Now, are they different, will you get two different diffraction patterns? No, because the integrated picture is nothing but instantaneous picture quantum mechanically. But then we are doing the experiment over finite time. Finite time means our timescale of the experiment is much larger than the time scales in the system.

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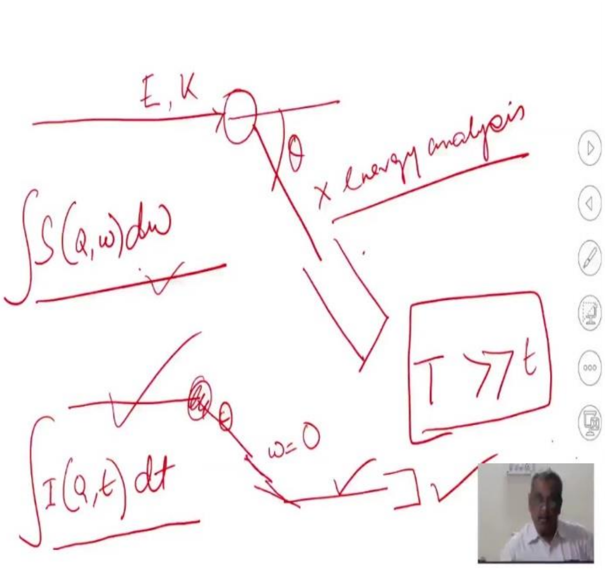

With this technique, we keep putting one frame, on another frame, and another frame, and another…. and that becomes a statistical average. On the other hand, when I do an experiment like this, where I do an absolute 0 energy transfer experiment that is equivalent to average over infinite time and these two things are exactly the same.

Statistical average at any instant over the entire ensemble of atoms taken one after another after another is the same as the statistical ensemble averaged over the entire time *t*. So, both of them are same, but conceptually they are slightly different.

Usually what we do is an integration of S(Q, ω) dω. And these are diffraction patterns. I am sure not whether many of you have used this concept, but this concept can be used in neutron scattering. And we do experiments in various ways. Conceptually it is possible to do it in two different ways.

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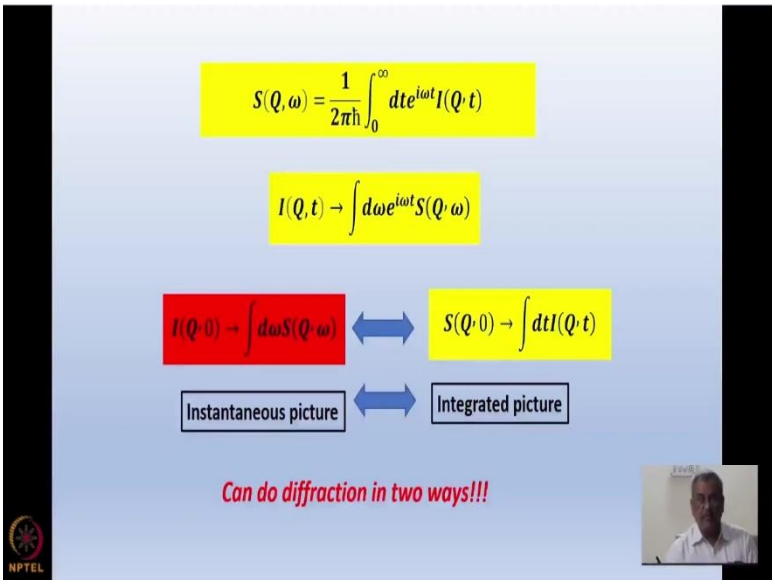

So, one is an instantaneous picture, and one is an integral picture, but both of them should converge to the same structure, otherwise, we are in trouble. And, both of them do convergence to same structure because the ensemble average and the time average for such a large number statistical system should be same.