Neutron Scattering for Condensed Matter Studies
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Lecture - 2
Calculating Neutron Scattering Cross-Section
Elastic Scattering

Keywords: Fermi Golden Rule, Fermi Pseudo potential, Scattering amplitude

In this lecture, we will be calculating the neutron scattering cross-sections, using the Fermi Golden rule. We discussed about neutrons in the previous lecture. I have mentioned all the desirable properties of neutrons that can be used for studying condensed matter structure and dynamics. And I also showed you the various experimental facilities like reactors and spallation sources that will be used. But today I will give you the theoretical background of neutron scattering cross-sections for neutrons using Fermi Golden rule.

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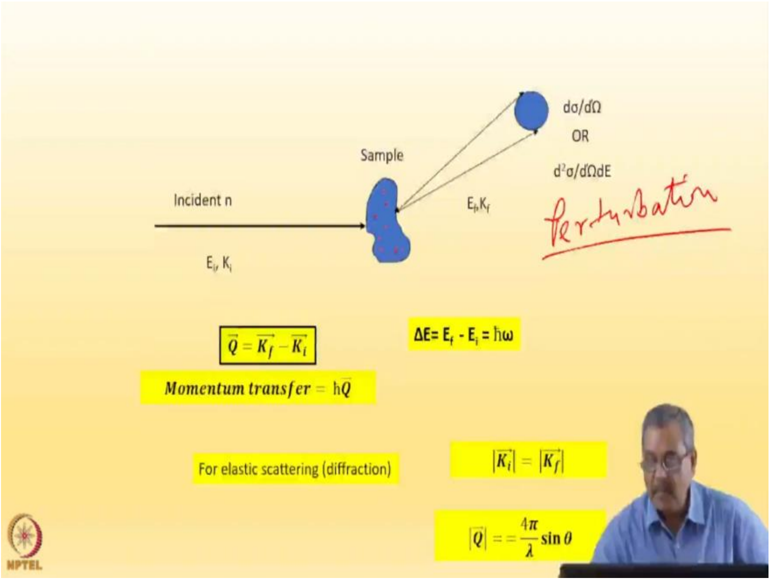

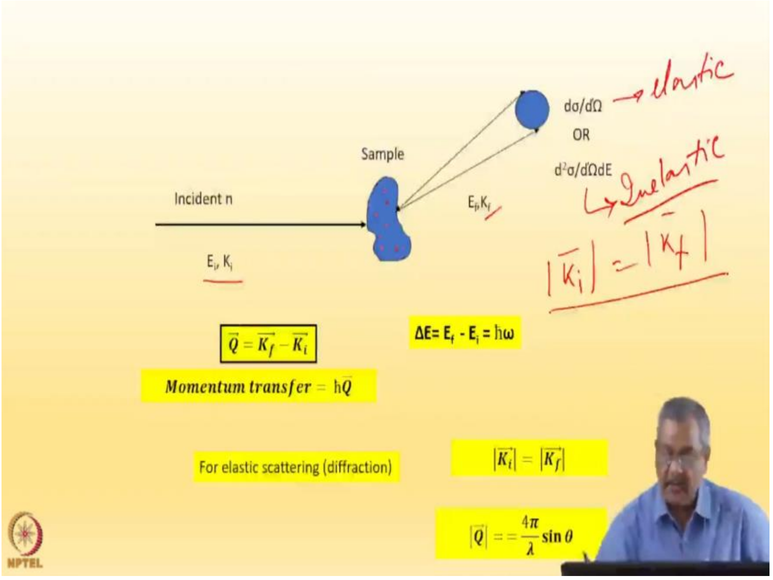

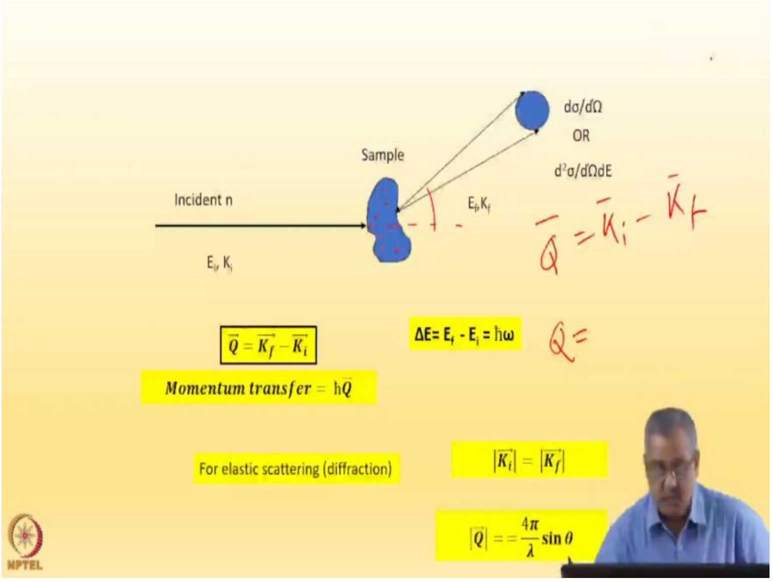

Here, the basic concept is that the sample is acting as a perturbation with its potential. There are atoms and molecules inside the sample and each of them do a perturbation for the incident neutron wave and sends it in some direction, either with the same energy or with changed energy. So, it can be $\frac{d\sigma}{d\Omega}$ when it is elastic. When it is inelastic, that means, there is an energy transfer, then it will be $\frac{d^2\sigma}{d\Omega dE}$.

This will encompass all sorts of scattering. So, fundamental premises are that, we have a sample in which we have atoms, molecules, all microscopic units that comprise the sample. And we have an incident neutron of energy E_i and wave vector $\mathbf{K_i}$. The sample perturbs this wave and sends it in a direction which is defined by the final wave vector **K_f**. And if it is inelastic, then there is a different energy; otherwise, it will be with the same energy. In the case of elastic scattering, the magnitude of **K_i** and **K_f** will be the same, but only directions are different.

So, this is the case of diffraction. Let me mention it at the beginning because when we bring in the formalism of Fermi golden rule, then I will use this elastic scattering expression; but it is equally true for inelastic scattering, which we will deal later. So, new direction, new energy (inelastic) or new direction only (elastic) $|\overrightarrow{K_i}|=|\overrightarrow{K_f}|$. And the wave vector transfer is given by $\vec{Q}=\overrightarrow{K_f}-\overrightarrow{K_i}$. If I miss the vector sign, then please excuse me; sometimes I tend to miss while writing, but they are all vectors.

Basically, these two vectors define the direction of the incoming neutron and the direction of the outgoing neutron. And Q is called as wave vector transfer. Often, we also say momentum; but it is not momentum, ħ.Q is the momentum transfer. Q for an elastic experiment, if the scattering angle is 2θ, then Q is given by

$$Q = \frac{4\pi}{\lambda} sin\theta.$$

That is the magnitude of Q for an elastic scattering in case of diffraction.

Hence, diffraction signifies that the length of the momentum or the wavevector remains same. So, with this let me take you to the formalism.

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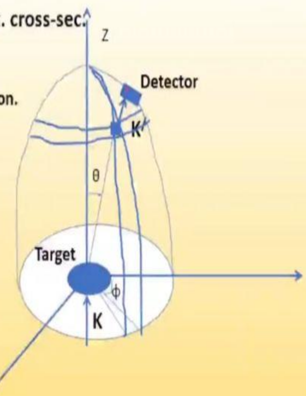
General expression for neut. scatt. cross-sec.



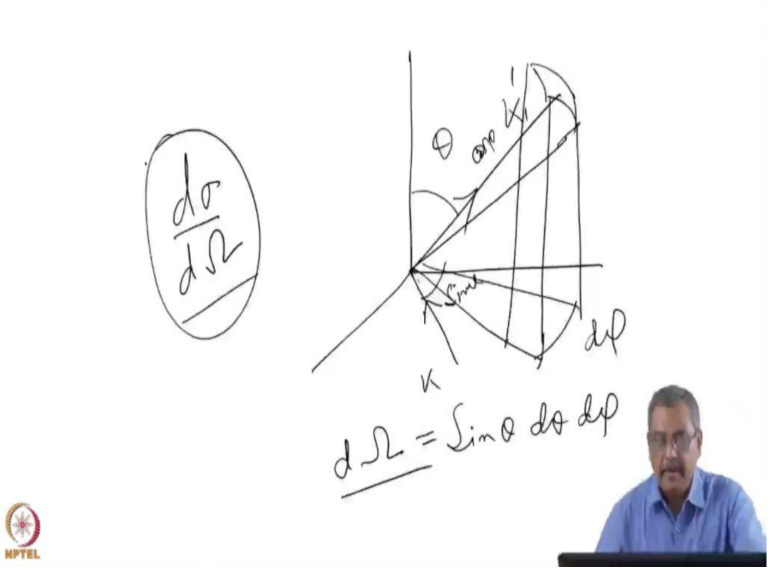
It is elastic K and K/ only differ in direction.
Energy remains same

If 'N' is the flux of incident neutrons,
n/unit area/unit time

Neutron scattered in to the solid angle

Given by: $N\frac{d\sigma}{d\Omega}d\Omega$

$$d\Omega = \sin\theta d\theta d\varphi$$



In general, what we are trying to define, let me just draw it for you. In the 3-dimensional space let us call it, the direction $\mathbf{K'}$. The neutron comes in some direction $\mathbf{K}$ and then it is scattered in this direction. So, in this direction ($\mathbf{K'}$), I can define a solid angle; and we know that solid angle will be given by the angular components here. So, here if it is θ, then this is $\sin\theta$, and $\cos\theta$. And this angle is given by dφ. Then the solid angle is given by sinθ dθ dφ. and normally the nomenclature is dΩ.

We are trying to evaluate the number of neutrons scattered per unit solid angle in the direction Ω. This is $\frac{d\sigma}{d\Omega}$. That is what we will try to evaluate in our formalism. This is the target and this is the solid angle, we assume that we have put a detector here in our theoretical approach. I am doing for elastic neutron scattering; so $\mathbf{K}$ and $\mathbf{K'}$ only differ in direction, their magnitudes are same. And then if N is the incident number of neutrons per second, then $N\frac{d\sigma}{d\Omega}$ multiplied by dΩ gives me the number of neutrons per second coming into the detector. But the solid angle is given by sinθ dθ dφ.

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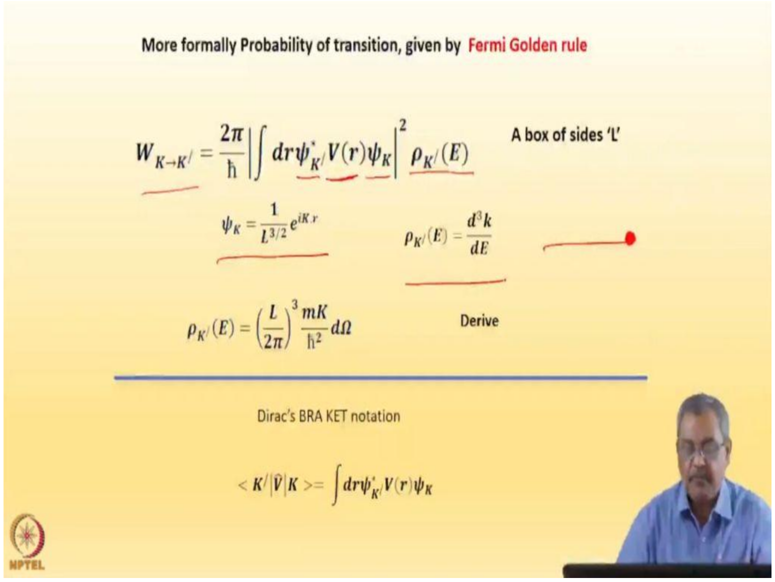

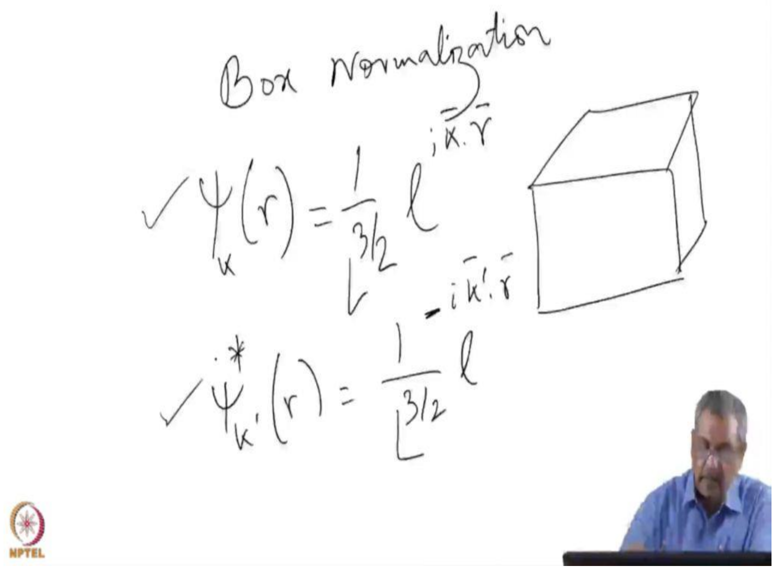

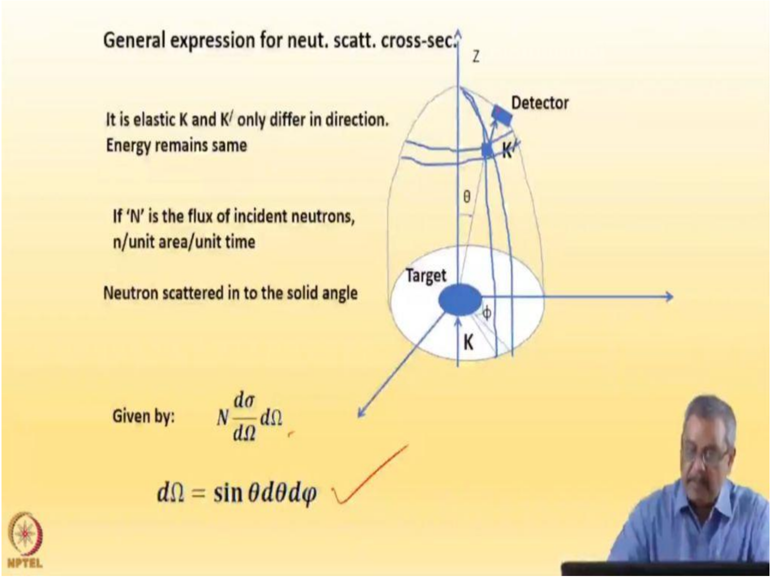

Now, let me go to Fermi Golden rule. Fermi Golden rule is about going from a state ψ_K under the perturbation by the potential V(r) to a state $\psi_{K'}$. And then this is probability amplitude, square of that will give me probability. This is the density of states at K′ at energy E. Usually, if it is inelastic, then this E will differ; but here, E is same for the incident and the outgoing neutron. And this gives me the probability of transition. Now, let me just show you that for neutrons we do a box normalization. You must be familiar with box normalization; because it is a plane wave we take and the plane wave does not decay anywhere.

We consider the plane wave is limited within a box of side L. In that case, the wave function ψ_K is a plane wave function. So, with normalization component $\frac{1}{L^{3/2}}$, I will write it as as $\psi_K(\mathrm{r}) = \frac{1}{L^{3/2}}e^{iK.r}$. And the normalization component is $L^{3/2}$ because, we force the neutron to be inside a box of size L. And then of course, we can make L to go to infinity. Similarly, $\psi_{K'}$ is written as, $\psi_{K'}(\mathrm{r}) = \frac{1}{L^{3/2}}e^{iK'.r}$.

Hence, ψ_K is the plane wave that is coming in and $\psi_{K'}$ is the plane wave that is going out. For the complex conjugate of these waves, everything else remains the same only the i goes to -i. So, this is the expression of the neutron waves coming in, neutron wave going out; and then in between ψ_K and $\psi_{K'}$, I squeez the potential V(r), which is the interaction potential between the neutron and the target nuclei let us say.

Now, I will evaluate the density of states $\rho_{K'}(\mathrm{E})$.

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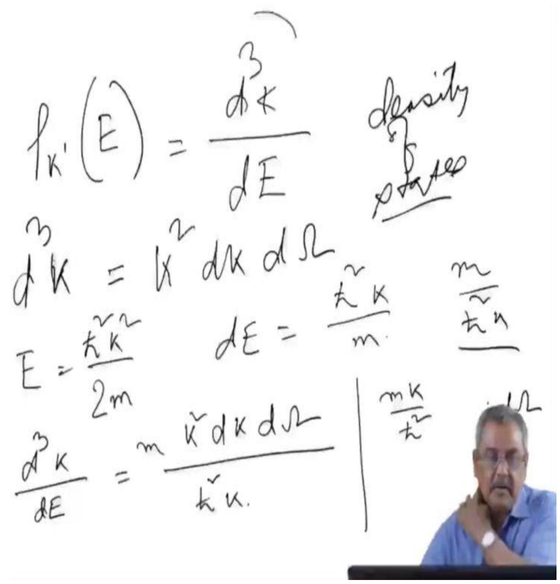

$\rho_{K'}$ at energy E is given by, $\rho_{K'}(\mathrm{E}) = \frac{d^3k}{dE}$, that means, the number of states that are available at energy E, here, E is same at wave vector $\mathbf{K'}$ and that is the density of states. Basically, the probability depends on two things. One that the probability amplitude quantum mechanically going from ψ_K to $\psi_{K'}$, under the action of potential; and the neutron is dictated by this density of states.

Now, d^3K is a small volume in K-space just like real space it is $k^2 dK\, d\Omega$; and $d\Omega$ is a direction which I described to you earlier. $E = \frac{\hbar^2 k^2}{2m}$, so, dE will be equal $\frac{\hbar^2 k}{m} dk$. Hence, substituting d^3K and dE, we have,

$$\rho_{K'}(E) = \frac{mk}{\hbar^2} d\Omega$$

Now, the question is that what are the number of states here inside the box?

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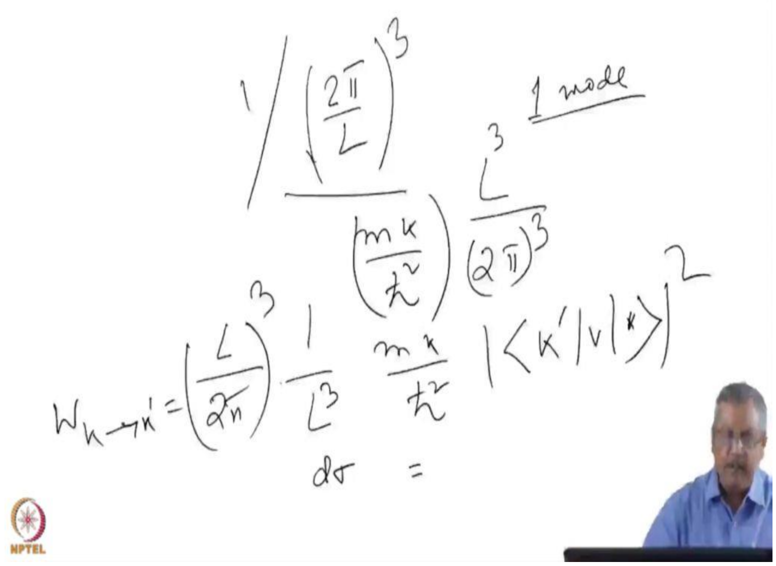
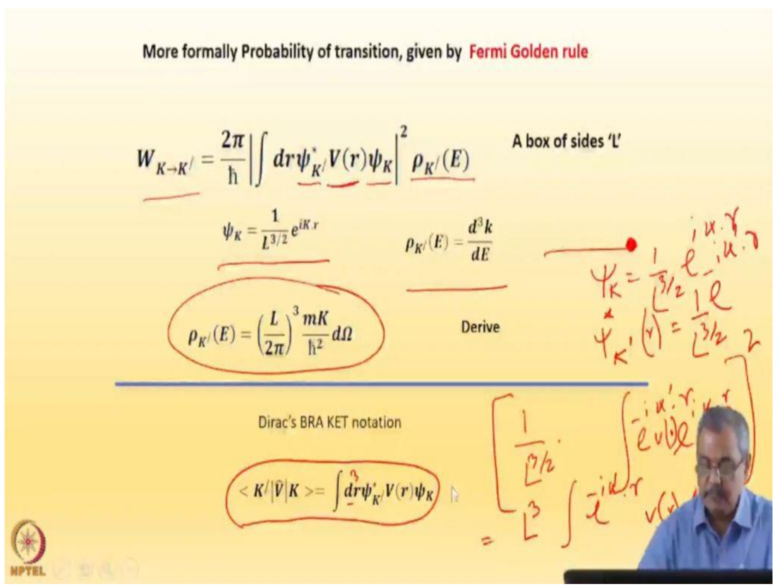
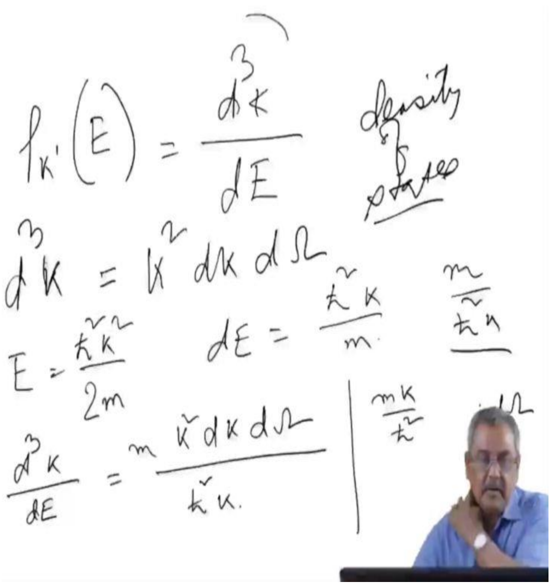

1 mode
$W_{k\to k'} = \left(\frac{L}{2\pi}\right)^3 \frac{1}{L^3} \frac{mk}{\hbar^2} |\langle k'|V|k\rangle|^2$
$d\sigma =$


More formally Probability of transition, given by Fermi Golden rule
$W_{K\to K'} = \frac{2\pi}{\hbar}\left|\int dr\,\psi^*_{K'} V(r)\psi_K\right|^2 \rho_{K'}(E)$
A box of sides 'L'
$\psi_K = \frac{1}{L^{3/2}} e^{iK.r}$
$\rho_{K'}(E) = \frac{d^3k}{dE}$
$\rho_{K'}(E) = \left(\frac{L}{2\pi}\right)^3 \frac{mK}{\hbar^2} d\Omega$
Derive
Dirac's BRA KET notation
$< K'|\hat{V}|K >= \int dr\,\psi^*_{K'} V(r)\psi_K$



So, now if the size is L, then we know in one dimension there is one allowed k value in $2\pi/L$ size. Now, because it is 3-dimensional box, so I will have a small volume in K-space, which is $(2\pi/L)^3$ which gives me 1 mode. Now in d^3k/dE gives me the available numbers of K values that is given by the density and this volume, which is $\frac{mk}{\hbar^2}$ which I found just now and gives how many numbers of allowed k values are there.

$(2\pi/L)^3$ is the basic volume, so, I have to multiply by density and; that is, $(L/2\pi)^3$. Now I have this expression and this is a $\rho_{K'}(E)$ which I calculated just now. This is the density and d^3k/dE gives me $\frac{mk}{\hbar^2} d\Omega$; $d\Omega$ is the solid angle. So, now, here if I put in $2\pi/\hbar$; and now, the wave function ψ_K is given the $\frac{1}{L^{3/2}} e^{iK.r}$; and $\psi^*_{K'} = \frac{1}{L^{3/2}} e^{-iK'.r}$.

Here then I have, when I input this over here $\psi^*_{K'} V(r) \psi_K$, what I have got here is $1/L^{3/2}$ into $1/L^{3/2}$ Then, there is an integral of $e^{-iK'.r} V(r) e^{iK.r}$ d^3r and then there will be the square of the whole thing. So, I will get L^3 here and this integral, which I can also write in a bracket notation as this.

This is d^3r; a volume integral and I can write it in a bracket notation. Now I have got $(L/2\pi)^3 (1/L)^3 (mK/\hbar^2)|\langle K'|V|K\rangle|^2$. The probability of transition from K to K'. Now, I have got when I talked about number of neutrons going in solid angle $d\Omega$, $d\sigma$, this will be scaled with respect to the flux.

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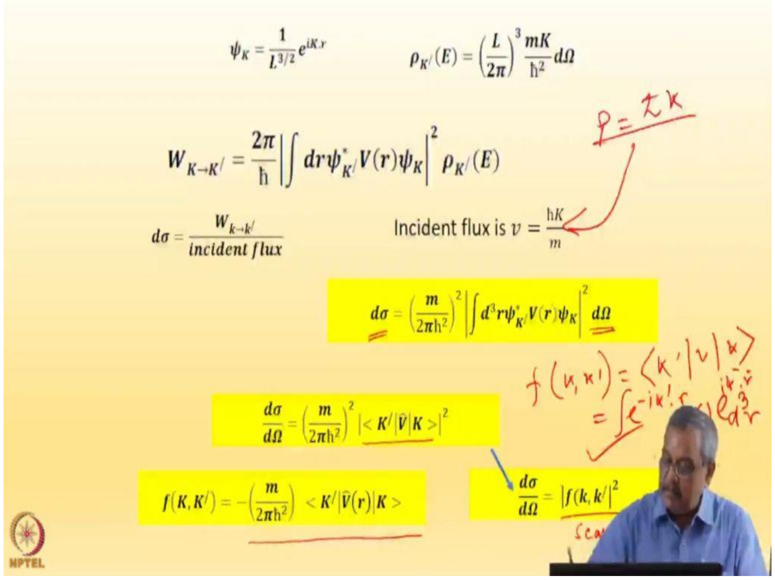

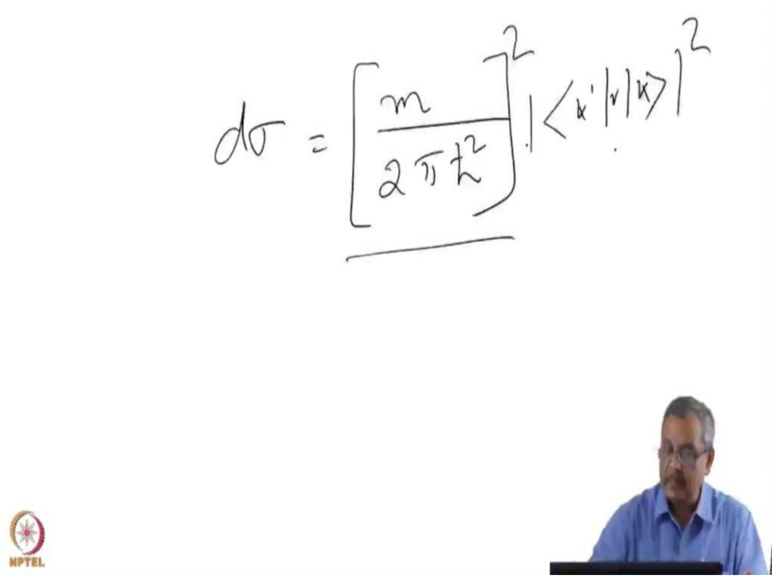

Please note that this (dσ) will be given by $W_{K \to K'}$ divided by incident flux; and P = ħK gives me incident flux ħK upon m. So, now the number of neutrons going in solid angle dΩ is dσ given by $W_{K \to K'}$ divided by incident flux.

Inputting all those things,

$$d\sigma = \left[\frac{m}{2\pi\hbar^2}\right]^2 |< K'|V|K >|^2 d\Omega$$

With the pre-factor.

$$\frac{d\sigma}{d\Omega} = \left[\frac{m}{2\pi\hbar^2}\right]^2 |< K'|V|K >|^2$$

Now, we can write this in terms of a scattering amplitude. We need scattering intensity per unit solid angle. We can write it in terms of a scattering amplitude, f(K, K`) defined as $\frac{m}{2\pi\hbar^2}|< K'|V|K >|$. And $\frac{d\sigma}{d\Omega}$ is given by square of f(K, K`) which is the scattering amplitude. So far I have not talked about the potential, but I have reached the formal expression for $\frac{d\sigma}{d\Omega}$, where <K`|V|K> is nothing but the integral of $\int e^{-iK'.r}V(r)e^{iK.r}d^3r$.

These are the neutron wave functions with the perturbing potential, integrated over the entire space; that means integrated over the entire sample. With this, I have reached an expression for number of scattered neutrons per unit solid angle in a certain direction.

Now, let me introduce the potential of interaction that is very important; because without that, we cannot go any far.

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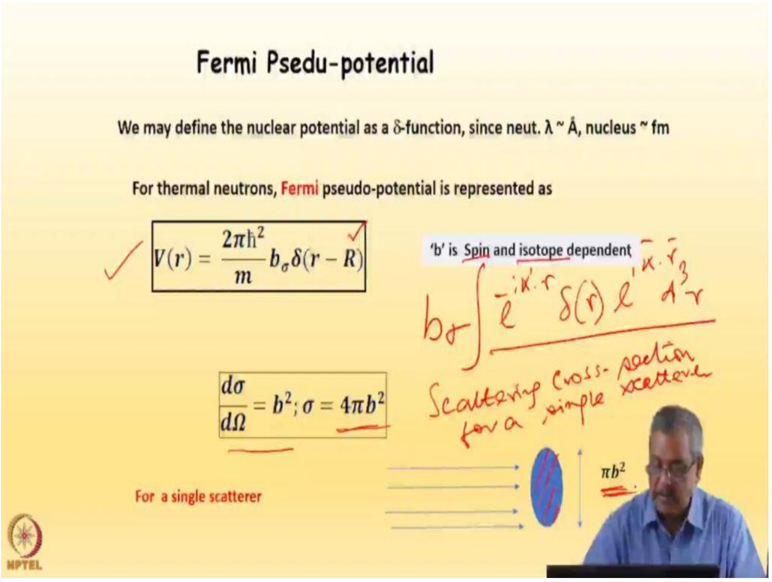

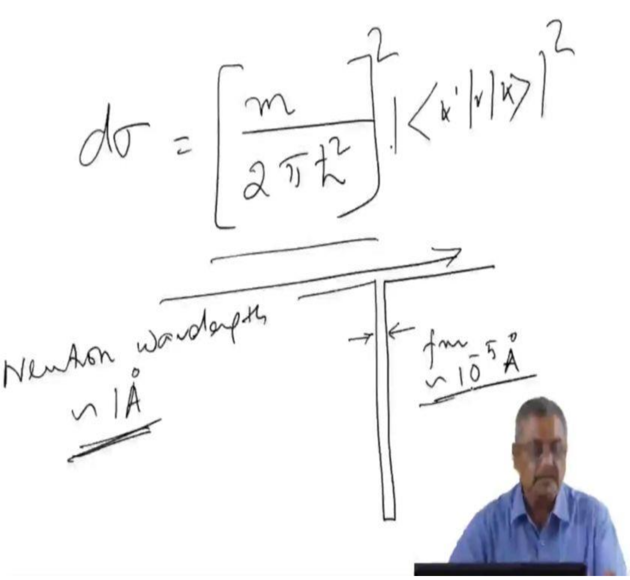

Here the term comes, Fermi pseudo potential. Why pseudo? Because here I am considering the neutron and the nucleus interaction. So, these are strong interaction, attractive interaction; that is why potential well is deep. It is extremely narrow why? Extremely narrow but there is nothing like qualitative expression of extremely narrow. What I mean is that the neutron wavelength, the thermal neutron wavelength is around angstrom. It can be 1 Å, it can be 5 Å it can be 0.1 Å. But, the extent of the nuclear potential is in femtometers, which is around 10^{-5} Å.

Now, I can say that this potential is infinitely narrow for this neutron of wavelength 1 Å. And then I can represent the nuclear potential as a delta function. This is what Fermi did and that is why this is named as Fermi pseudo potential. If you remember I had an expression before the scattering amplitude $\frac{m}{2\pi\hbar^2}$, to offset that, I introduced this constant $\frac{2\pi\hbar^2}{m}$ so that they cancel with each other; and it is a constant term so that I can do it. And I also have a scattering amplitude b_σ. And then for one single scatterer sitting at point R is a delta function $\delta(r-R)$.

So, this is the expression for the Fermi Pseudo potential for a single scatterer. This scattering length is spin dependent and isotope dependent where, the scattering amplitude signifies the interaction between a neutron and the nucleus. So, that is why it depends on the spin of the neutron; and the spin of the nucleus and its orientation with respect to the neutron spin. That also depends on the isotope because the nuclear spin changes with isotopes; hence it is isotope dependent and spin dependent.

But, one thing is there. Now you can see if I write $e^{-K`.r}$ $\delta(r)$ $e^{K.r}$ and then b_σ; because if there is only one nucleus, I can put it at origin. This term gives me 1 because r = 0 and this is 1; so, this gives me b_σ. So, the constant factor $\frac{m}{2\pi\hbar^2}$ cancels with $\frac{2\pi\hbar^2}{m}$. So, $\frac{d\sigma}{d\Omega}$ is b^2 and $\sigma = 4\pi b^2$ is my scattering cross section for a single scatterer.

And then you can see that if I consider it classically, it should have been πb^2; but here because it is on solid angles, it is $4\pi b^2$. This is just a classical picture of what you mean by scattering cross section in the beam path; you have a disk of size b and then it is given πb^2 the area of the disk. Here it is $4\pi b^2$ for a single scatterer. But now, let us take an assembly of scatterers and what happens then?

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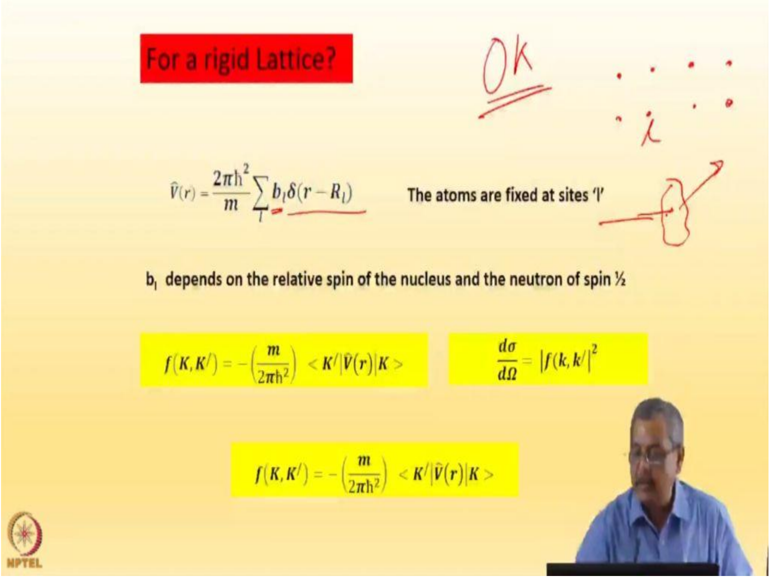

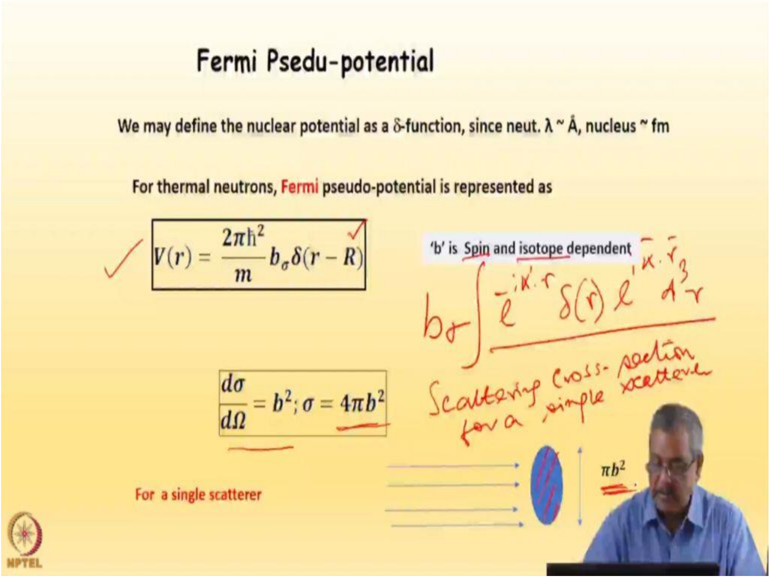

Let us consider a rigid lattice. Rigid lattice means I have taken out the dynamics from the lattice. So, it is a lattice at 0 K and there is no dynamics and the atoms are fixed at the sites. So, just now I said the for a single atom it is δ(r-R); but now, my atoms are fixed at these sites. A general site, I can call it l^{th} site; and then the potential is a sum of these delta functions. Each site has got a scattering length of b_l because I have not said what is the spin or what is the isotope at that site. So, in general, it is a site dependent scattering length b_l and $\delta(r-R_l)$.

This gives the sum over all the sites that gives the potential offered by the sample to the neutron in this neutron scattering experiment. Now, let me show you that I wrote $f(K, K`) = \frac{m}{2\pi\hbar^2}|< K`|V|K >|$; and $\frac{d\sigma}{d\Omega}$ is given by this.

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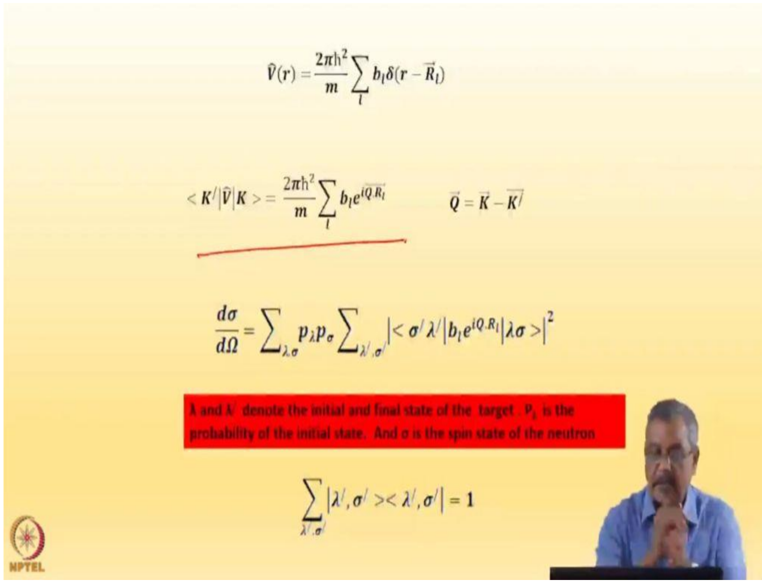

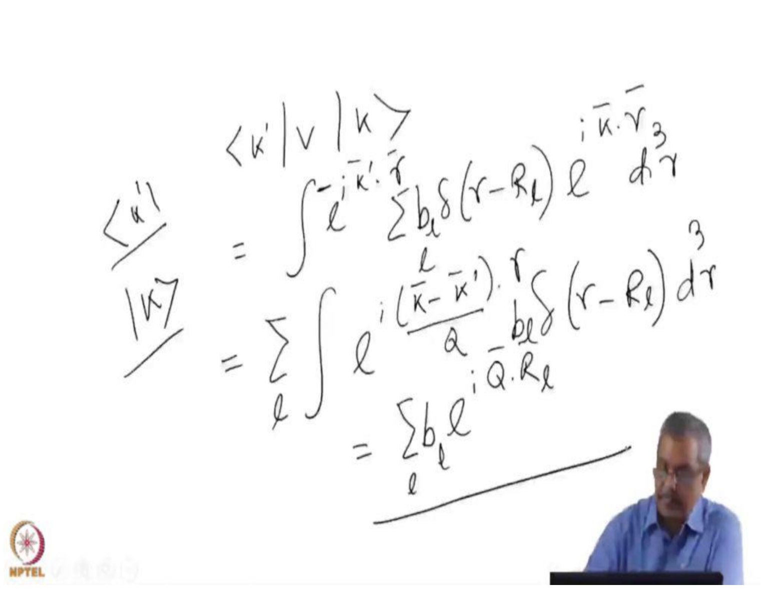

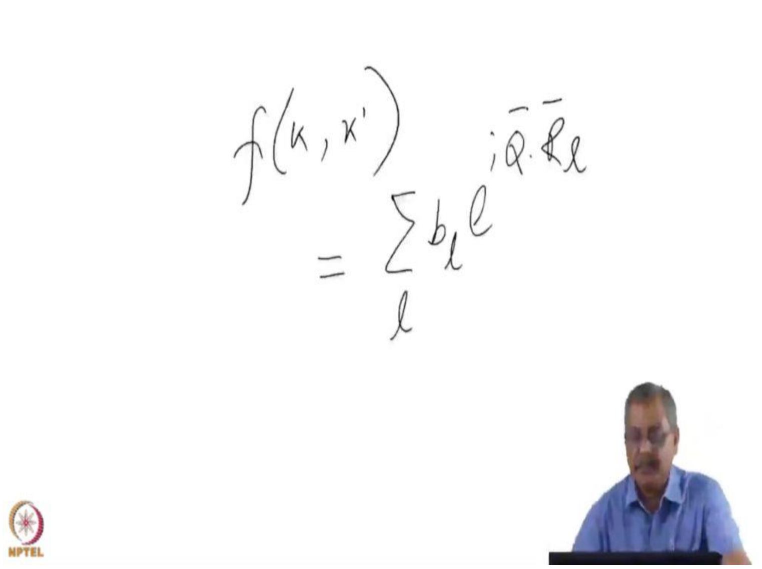

Now let me do these summations. V(r) is nothing but sum of delta functions. Earlier I put the single scatterer at the origin; now you cannot do that. So, now <K`|V|K> is equal to $e^{-iK\prime.r}$, because this is complex conjugate -bra and ket- this is complex conjugate and this is the wave function, then there is a sum over l $\delta(r-R_l)$; because I have to add up over all the sites in the lattice, sum of them over ‘l’. Then, $e^{iK.r}$and then integral over d^3r.

So, I can write as $e^{-i(K-K\prime).r}$ $\delta(r-R_l)$ d^3r and I take the summation over ‘l’. This is nothing but the wave vector transfer Q; so, this is equal to sum over ‘l’ $e^{-iQ.R_l}$. Now, r R_l, Rl summation over l; sorry I forgot to put the b_l over here. The b_l has to be there which is the most important term so b_l with summation over l. So, now my scattering amplitude f(K,K`) is $\sum_l b_l e^{iQ.R_l}$.