Neutron Scattering for Condensed Matter Studies
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Week 02
Lecture 04B

Keywords: Dynamics, operators, ensemble, Maxwellian distribution, delta function

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Now, I will introduce dynamics in the formalism.

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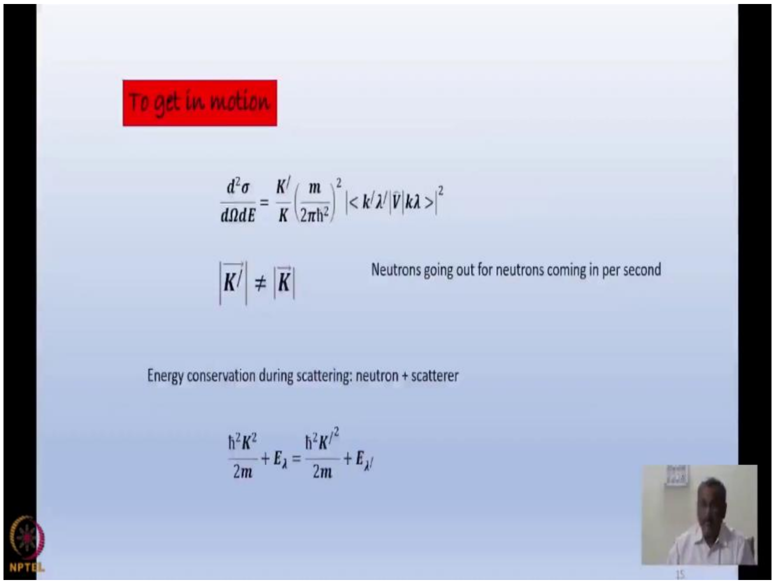

I request you to recall that we had been working to calculate the scattering amplitude, where we evaluated the effect of potential on the incoming and outgoing wave vector of neutron. Now, when we talk about inelastic scattering, there is energy transfer between the neutron and the scatterer, and neutron and the scatterer together form a total system.

Then the magnitude of the scattered vector K' is no more equal to K, which was true for the diffraction case. So, I need to put a factor of $\frac{K'}{K}$, because I have to compare the number of neutrons going out for neutrons coming in per second and that is given by the magnitude of $\frac{K'}{K}$.

Also, if there is energy exchanged between the neutron and the scatterer, then there should be an energy conservation during scattering, that means, the energy of the system E_λ and the kinetic energy of the neutron, in nonrelativistic limit which is $\frac{\hbar^2 K^2}{2m}$ must be equal to $\frac{\hbar^2 K'^2}{2m}$ + energy of the scatterer after scattering.

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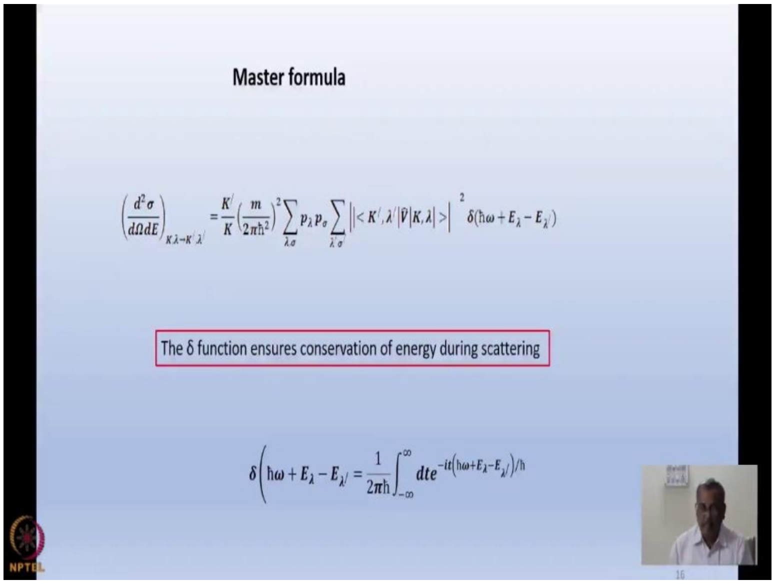

These are the energy constants. So, I will write down a long formula, but in the same way what I did earlier, I will go slowly on this and derive it.

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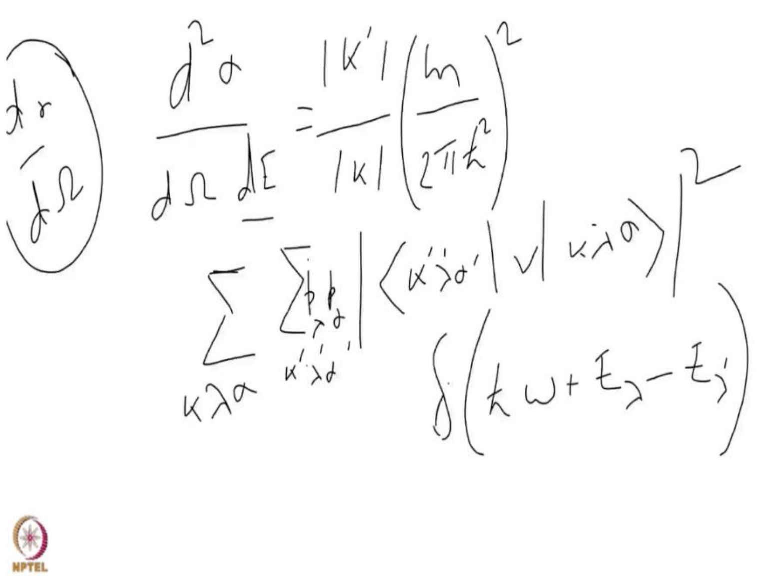

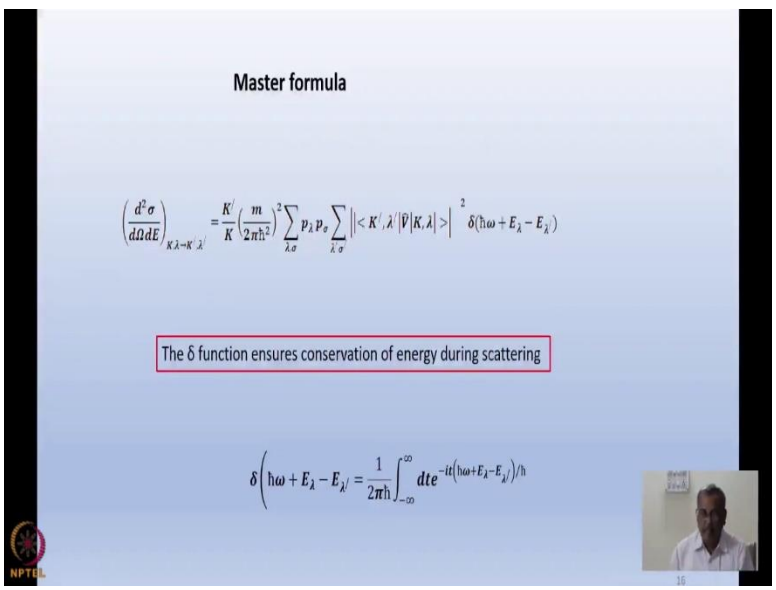

Now, I am writing the scattering cross section as $\frac{d^2\sigma}{d\Omega dE}$, means number of neutrons per unit solid angle per unit energy interval. First there is flux normalization. So, neutrons coming in versus neutron going out per second. I had this factor earlier also, if you remember, in this part.

I have to sum over initial states and also sum over final states. Then, I have potential V working on neutron of wave vector K, system energy E_λ and state σ, and square of that. And since I am taking all possible outgoing states, I have probabilities, p_λ p_σ. Now, in this expression I need to introduce a delta function which takes care of the energy conservation during scattering and it looks like $\delta(\hbar\omega + E_\lambda - E_{\lambda'})$, this is the energy difference of the neutron before and after scattering which should be equal to the energy difference of the system, because neutron can give or take energy and there should be a balance, what neutron gives is taken by the system, what system gives should be taken by the neutron. Hence, I introduce a delta function to say that in this scattering cross section, I have conservation of energy between neutron and the system.

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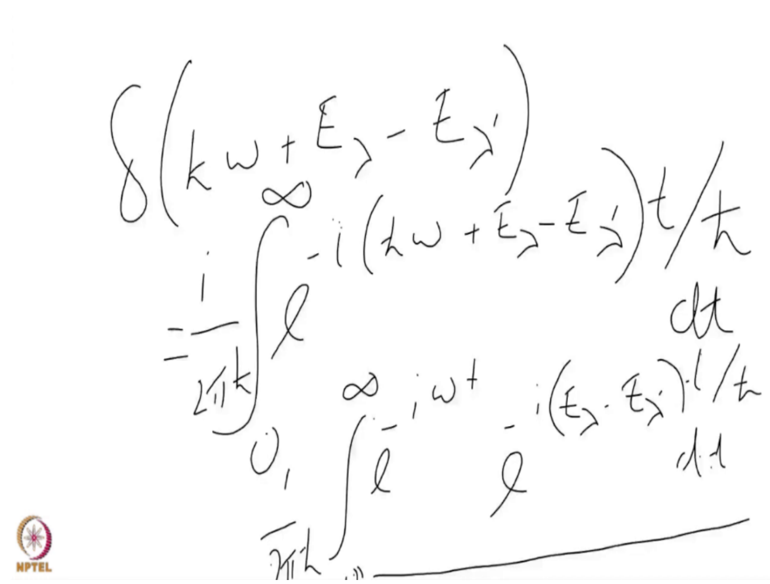

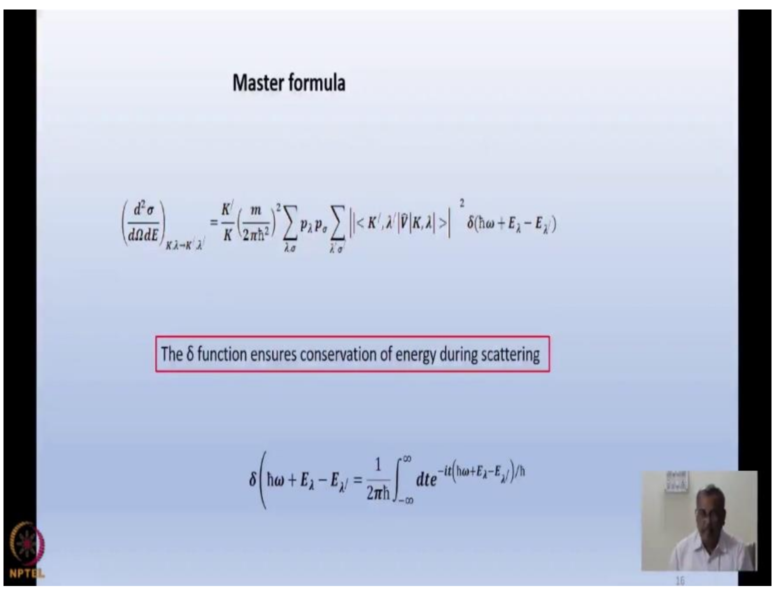

There are various ways of writing delta function and I use one of them, which is the integral form equal to $\int_0^{\infty} e^{-i(\hbar\omega + E_\lambda - E_{\lambda'})t/\hbar} dt$, this is an integral representation of the delta function in time domain. I can write this as, $\int_0^{\infty} e^{-i\omega t} e^{-i(E_\lambda - E_{\lambda'})t/\hbar} dt$

Now, I will insert this integral inside my statistical averaging the expression. This is what the expression for the delta function looks like, I missed this 2πħ a constant term and I will insert this delta function inside my ensemble average.

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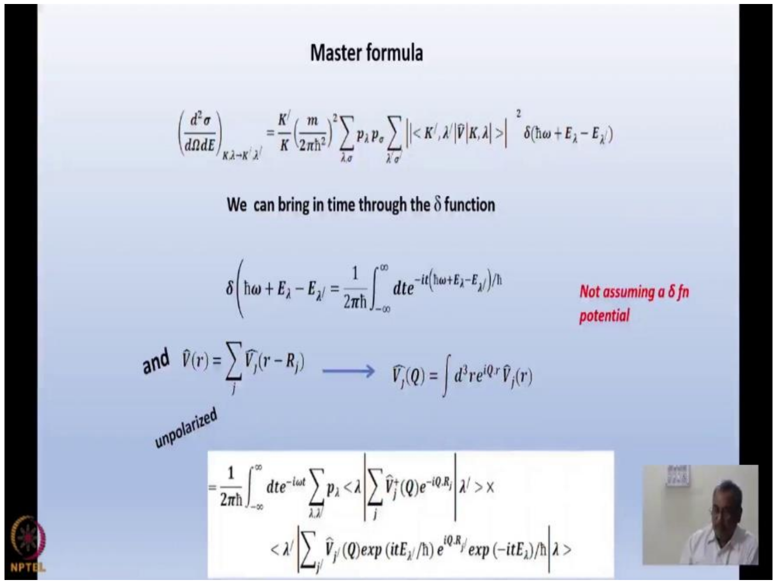

And now that I have written this part, we can bring in the time. I will also introduce a Fourier transform over the potential. Right now, I am putting the Fourier transform, we know that the Fourier transform will be $e^{iQ.r_j}$ for a delta function potential. But if I do not have a delta function potential, in general, then I can write down Fourier transform of the potential as $V_j(Q)$ that is the Fourier transform of the potential at site R_j and it is $V_j(Q)$ in Q space., I will write down the expression in which I have $K'.K$ and I know that it gives me $e^{i(K-K')}$, here K-K` = Q, and $\hat{V}_j$ is $e^{iQ.r}\hat{V}_j(r)$.

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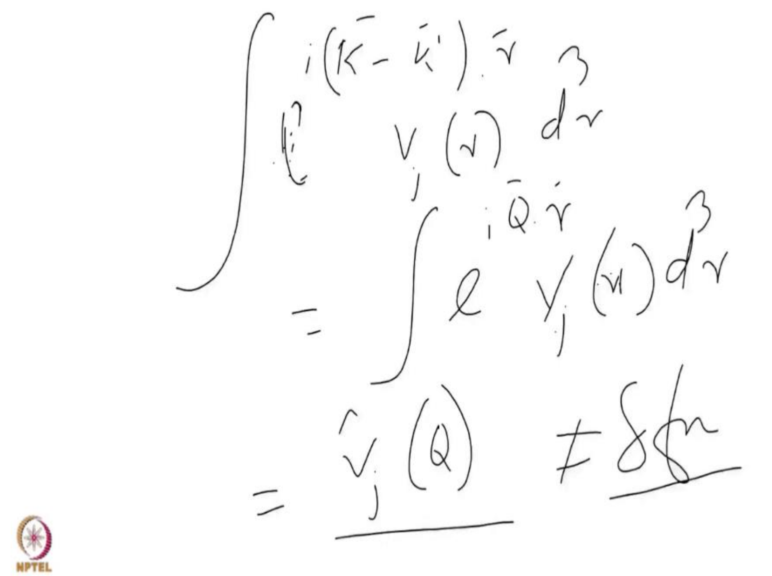

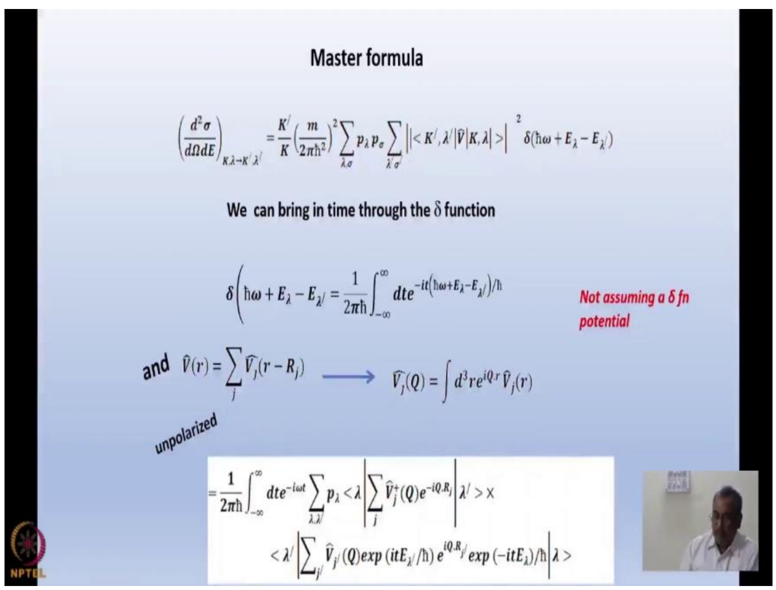

In summary,

$$\int e^{i(K-K\prime).r} V_j(r) d^3r \;=\; \int e^{iQ.r} \hat{V}_j(r) d^3r \;=\; \hat{V}_j(Q)$$

It gives me the Fourier transform of the potential. Right now, I am not assuming it a delta function, I can put delta function at any time and get back my simple expression. For the time being, I am not using that. Now,

$$\delta(\hbar\omega + E_\lambda - E_{\lambda'}) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{-i(\hbar\omega + E_\lambda - E_{\lambda'})t/\hbar}\, dt$$

So, I can write this, I have $\lambda, K, \sigma, \lambda', K', \sigma'$. This integral gives $\hat{V}_j(Q)$.

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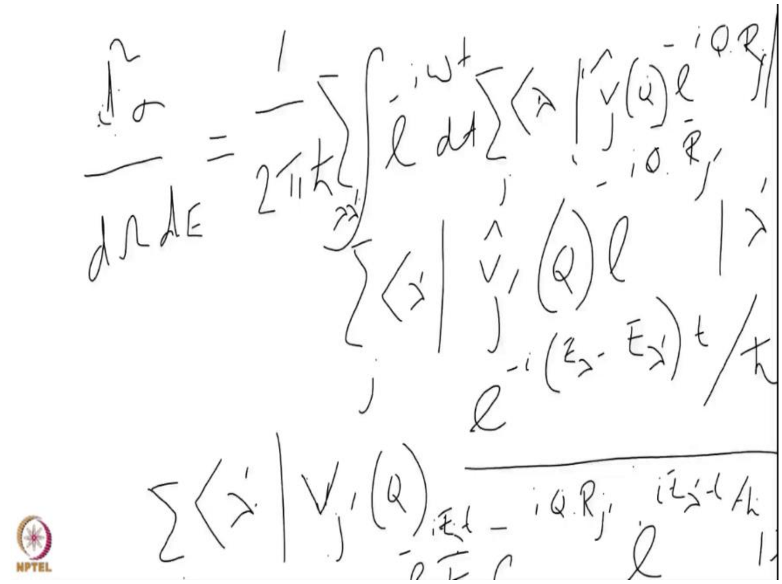

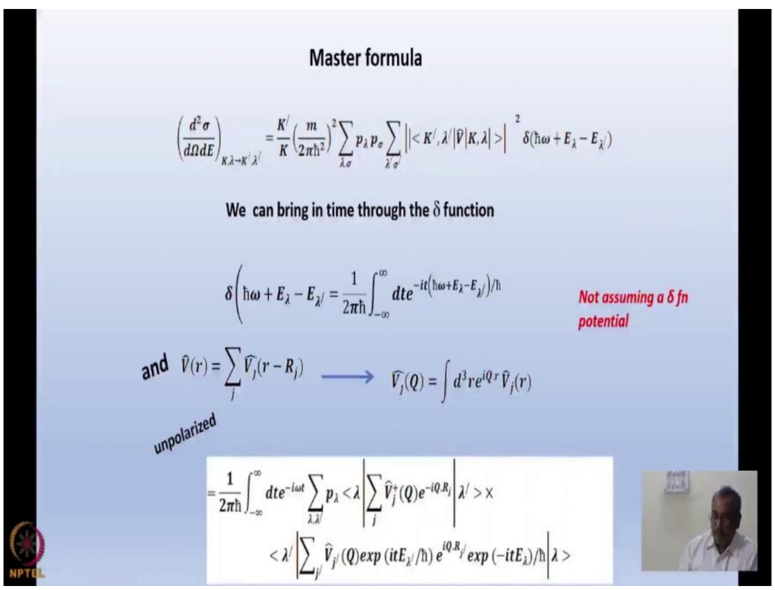

Including all these relations, the expression for scattering cross section becomes long. This is the first part. Now, we have summation over λ, λ'. This is a very long expression; I will go one by one. There are two brackets one complement of other, it starts with λ, λ'λ λ`, squeezed in between $V_{j'}(Q)$ and $V_j(Q)$, because there are two summations j and j`.

You can see there are two summations over λ, λ' λ λ`and there are two summations over j and j' There are two brackets we can play around, I can take them this way that way which allowed because these are just integrals, with physical values and we can use to move them along. With that I have got this expression and also, I have got $e^{-i(E_\lambda - E_{\lambda'})t/\hbar}$ and I have integration over time and $e^{-i\omega t}$.

Now, I will use this thing inside, that means, what I am going to do is' summation over j which is there,and λ' is also there. Now, this $e^{-i(E_\lambda - E_{\lambda'})t/\hbar}$ I put it inside this bracket. So, I write it like this inside the averaging bracket.

I have $e^{iQ.R_j}$, I bracket it with $e^{iE_{\lambda'}t/\hbar}$ and $e^{-iE_\lambda t/\hbar}$ and then rest of the things remain same. I have got a summation over λ and summation over λ' that means, over all possible initial states and over all possible final states. The integral over time remains. This is a very interesting thing.

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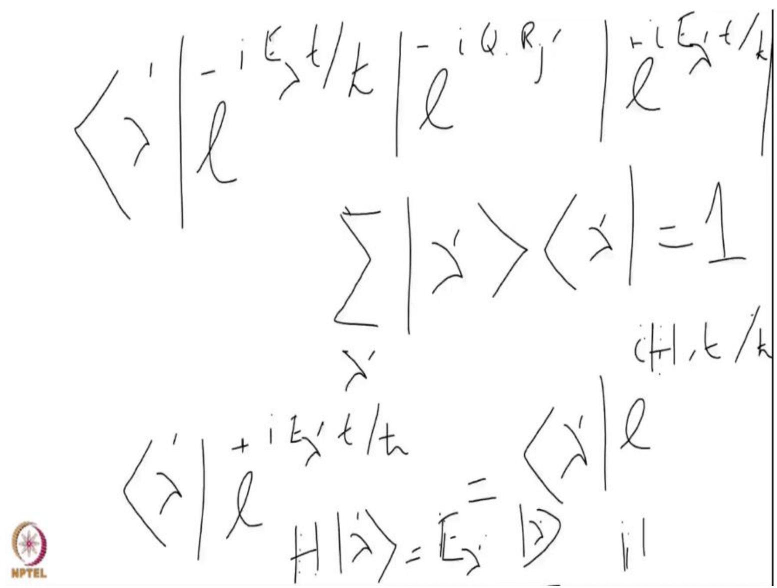

What I have done actually, if you see the expression is, $\left\langle \lambda' \middle| e^{-iE_\lambda t/\hbar} \middle| e^{iQ.R_j} \middle| e^{iE_{\lambda'}t/\hbar} \middle| \lambda' \right\rangle$. First we will use the fact that $\sum_{\lambda'} |\lambda'><\lambda'| = 1$ is like a projection operator and for any wave function the total projection is equal to 1 because, it is like sum of direction cosines equal to 1.

But now, you concentrate on this part that means, these terms, I can also turn it around I can bring this one to one side this one to other side. So, what happens you know $\left\langle \lambda' \middle| e^{iE_{\lambda'}t/\hbar}\right.$this is the same as $\left\langle \lambda' \middle| e^{iHt/\hbar}\right.$, because H operating on a state gives the energy of the state into wave vector, this is standard rule for Eigen functions of H in quantum mechanics and similarly H λ will be equal to E λ.

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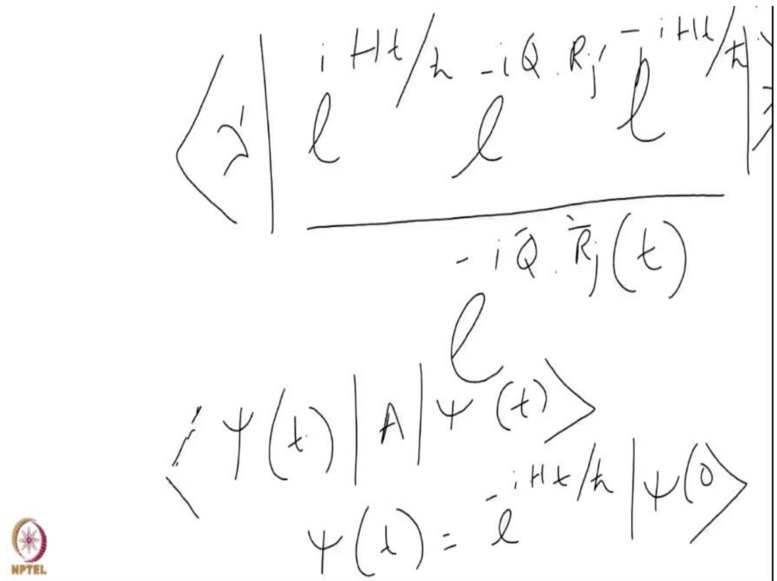

So, inside the bracket also I can write $\left\langle \lambda' \middle| e^{-iHt/\hbar} e^{iQ.R_j} e^{iHt/\hbar} \middle| \lambda' \right\rangle$. This basically gives me the time evolution of the operator. This is the biggest change now comes in. Why? Because we know the time dependence either you can put to the wave function or you can put to the operator.

Here, I am putting this time dependence on operator and we know for any static state, what is the time variation. For a wavefunction ψ the expectation value of a physical operator A at time t is given by, $\langle \psi(t)|A|\psi(t)\rangle$. Now, for stationary states, $|\psi(t)\rangle = e^{-iHt/\hbar}\,|\psi(0)\rangle$. That means, if I consider the base wave functions are unchanged then I can write the same thing as,

$$\left\langle \psi(0) \middle| e^{iHt/\hbar} A e^{-iHt/\hbar} \middle| \psi(0) \right\rangle$$

$$\langle \psi(0)|A(t)|\psi(0)\rangle$$

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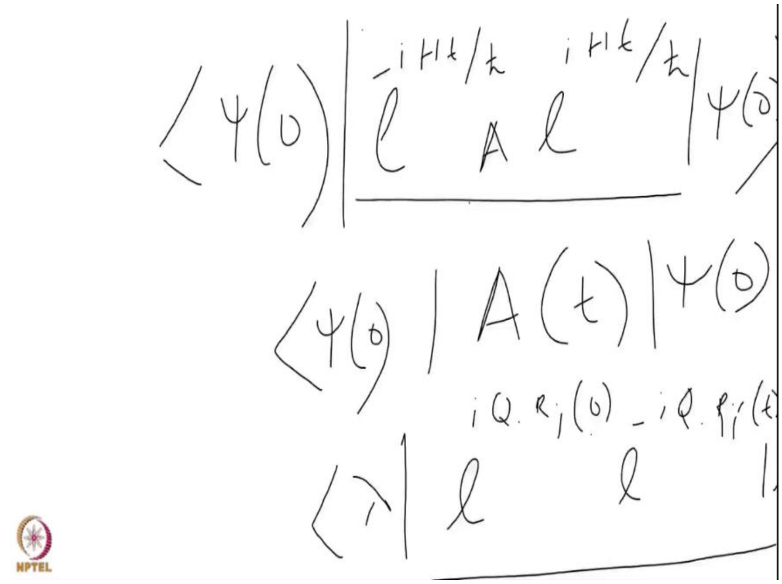

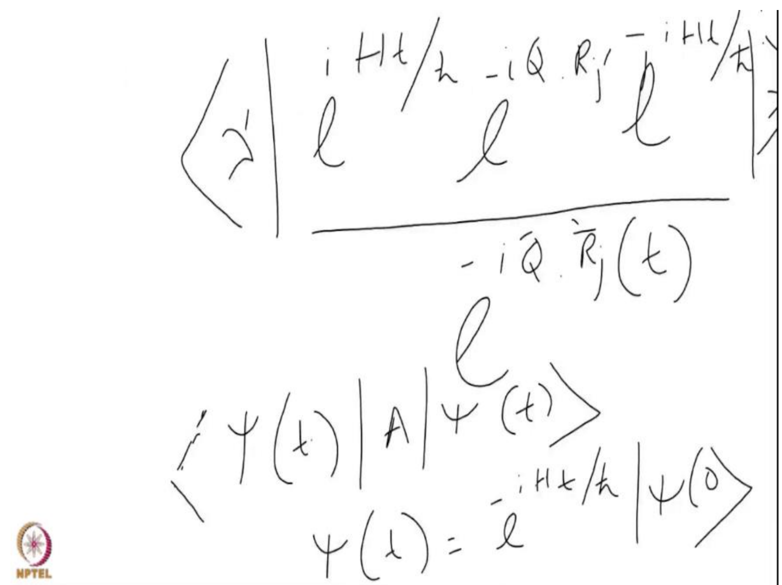

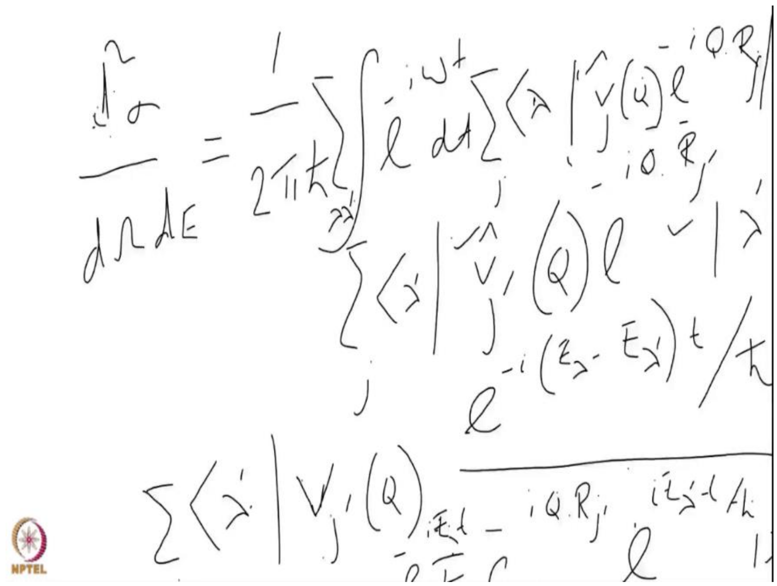

Hence, if the set of Eigen functions are stationary, then the time dependence is absorbed in the operator. And I can find out the average at any time using this expression and that is what I have done over here. So, I could write it as $e^{iQ.R_j(t)}$ instead of $e^{iQ.R_j}$. I have brought in the time dependence of position vector in this. Let me go back.

I introduced a delta function to conserve energy in the scattering process, then I use a specific expression or representation of delta function in terms of time integral because it is in the energy space, then I also introduced the Fourier transform of the potential.

Now, I had input this in the large expression where I have put the $e^{-i(E_\lambda - E_{\lambda'})t/\hbar}$ from the integral over time inside the bracket for $V_{j'}(Q)$ and that gives me $R_{j'}(t)$, because I showed you that for any operator the time dependence is given by $e^{-iHt/\hbar}$ into the operator ,with the wave function which is stationary. So, either we can take the time dependence on the wave function or on the operator, here we take a stationary set of wave functions and the operator is changing and that is how we get the expression.

If I take it out sum will remain for λ for the other things and I get out the average outside. You can see that I have done the same over here in that summation I had probability p_λ of state λ, if I consider the summation over λ, λ'over all the projections then I can remove the summation over λ' because summation over λ'`, summation gives me 1.

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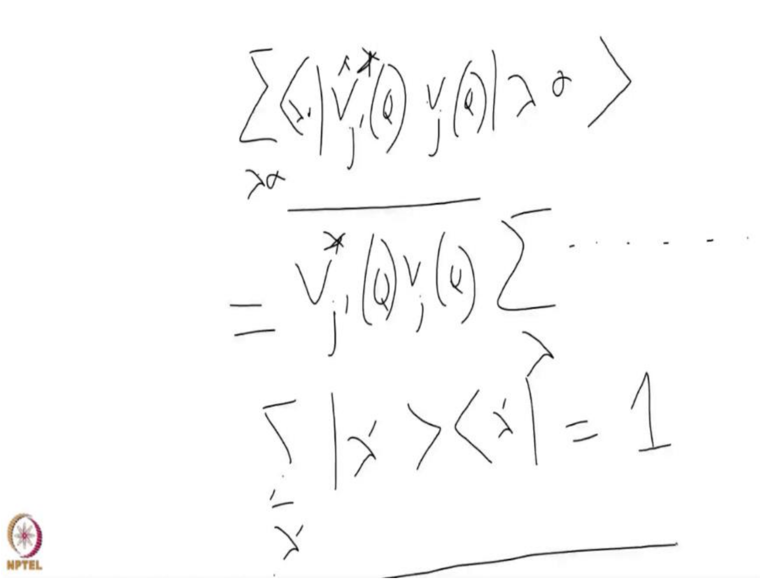

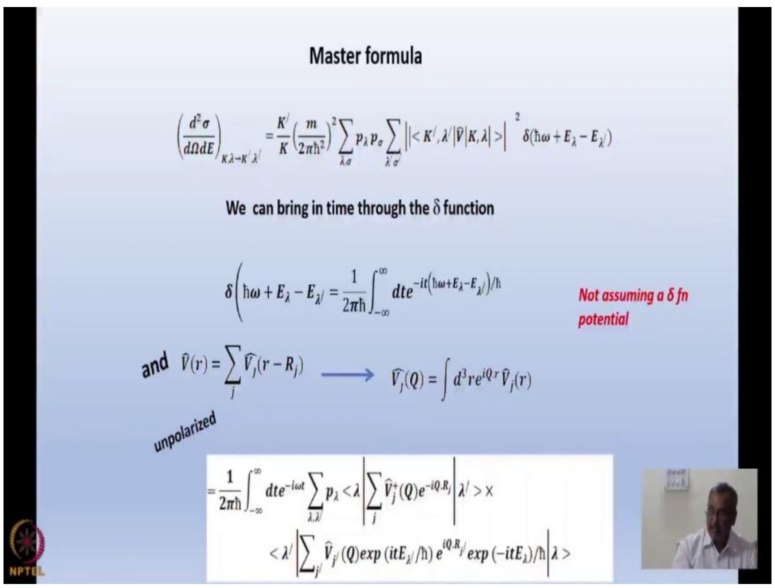

So, that summation I am removing from there, I have brought in $e^{iE_{\lambda'}t/\hbar}$e and $e^{-iE_{\lambda}t/\hbar}$, from the integral you see for delta function inside the summation sign and inside the ensemble average picture.

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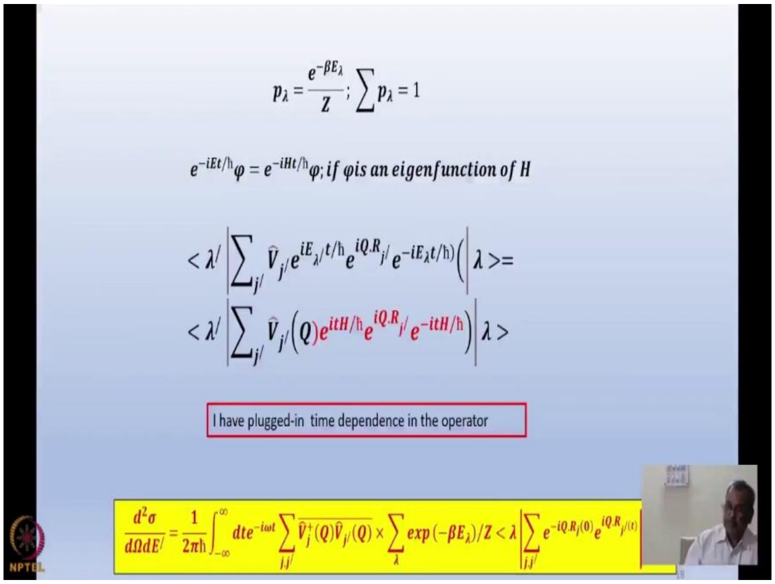

When I do that, there are two things, one is that in the classical picture which will be valid for most of the cases, the probability of energy E_λ given as a Maxwellian distribution which is $\frac{e^{-\beta E_\lambda}}{Z}$. And this part I will emphasize once again for any wave function, you can see if ϕ is an Eigen function of the Hamiltonian which is λ here, part in red, I told you that this gives the time dependence in the operator variable R_j.

Now, I can write down the expression, it is a Fourier transform over this whole part where we have a summation over all the sites for the Fourier transforms at specific sites, this is a p_λ, which is a statistical weight for the state with energy E_λ. And there is an averaging of $e^{-iQ.R_j(0)}e^{-iQ.R_{j'}(t)}$. This is an ensemble average of and summation over all the atoms. What does it mean physically.

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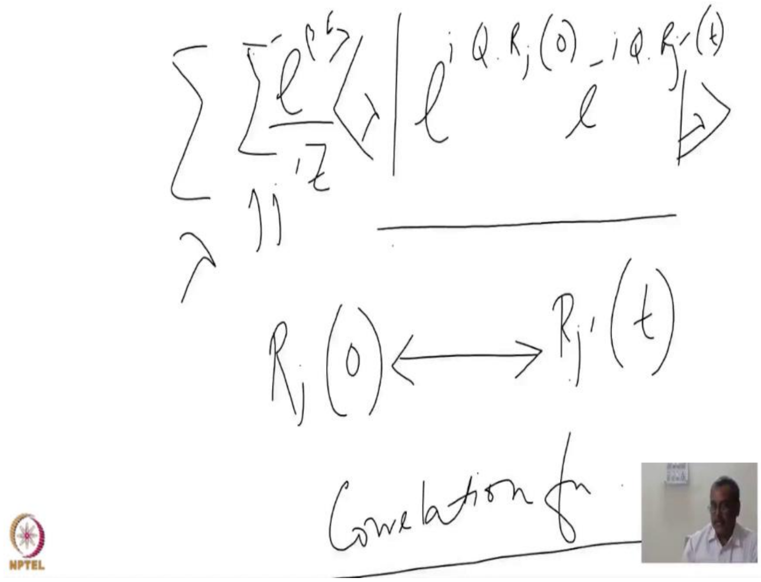

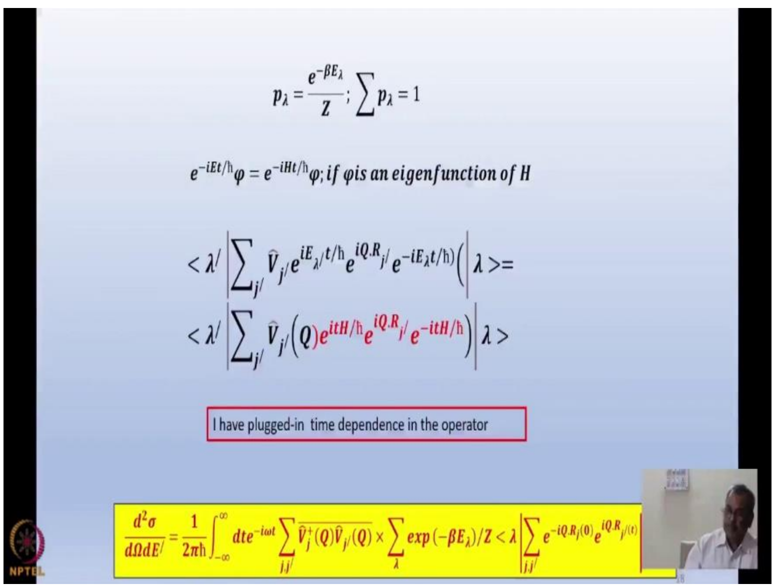

I have a summation over jj'`. I have got an ensemble average of $e^{-iQ.R_j(0)}e^{-iQ.R_{j'}(t)}$. One is that we have the energy E_λ of the state λ, the probability of that state is $\frac{e^{-\beta E_\lambda}}{Z}$, where Z is partition function. We are aware that this is the Maxwellian weight, $e^{-E/kT}$ upon sum over all the states.

And this part is about dynamics of the system. Why? Because I am seeking the ensemble average of a quantity, which has, I am stating, if the j^{th} atom is at the origin at time t equal to 0, what is the position of the j' atom at time t under the given dynamics? It correlates the two positions at two times, and this is called a correlation function.

This correlation function is directly related to the double differential scattering cross section, $\frac{d^2\sigma}{d\Omega dE}$. So, you can see the double differential scattering cross section is given by the time Fourier transform over a large expression in which I am looking at the ensemble average probabilistically weighted with the energy $\frac{e^{-\beta E_\lambda}}{Z}$ is a statistical way and I am seeking the average value, ensemble average value of one atom, molecule….. whatever it is, at one site and what is the probability of another scattering unit at a different site and time? I call it in general scattering unit at another site at time t. If there is no correlation, then we can take them out of this average separately, we can do the averaging separately, and then ensemble, I can tell, but if they are correlated, for example, phonons in a solid, motion of one is related to the motion of another one and then the ensemble average needs to know the correlation to get the double differential scattering cross section.

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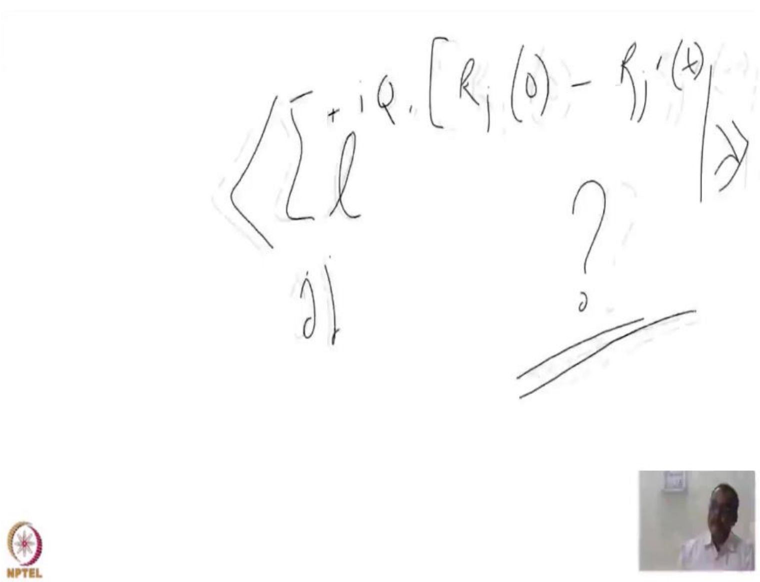

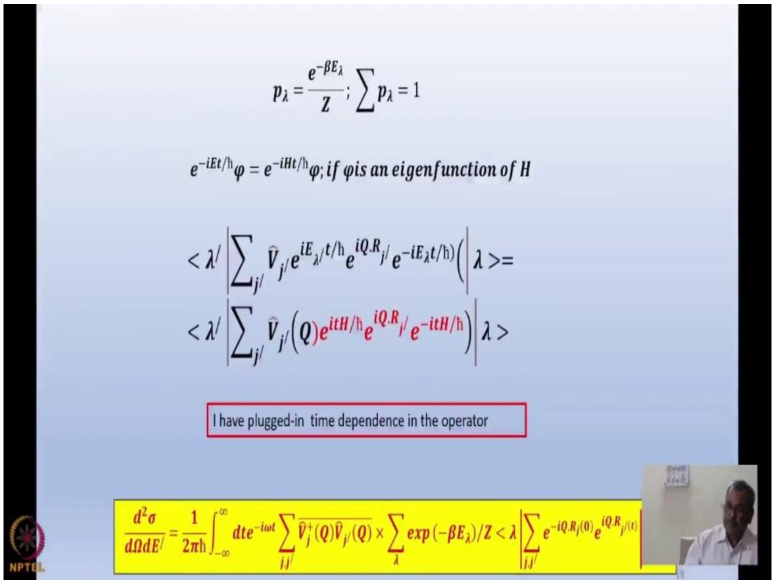

I have not given any prescription to find out the ensemble average and summation over all sites. If we want to know the double differential scattering cross section, we do need a prescription how to calculate that. In next part and later, I will give you at least some prescription because there are various kinds of dynamics.

But know that I have to have a prescription to figure out how to calculate $[R_j(0) - R_{j'}(t)]$. Either I have to do a modelling because direct Fourier transform is often not possible. But what I want to highlight to you that time Fourier transform over this large quantity on the right-hand side you see, gives me $\frac{d^2\sigma}{d\Omega dE'}$ that means number of neutrons per unit solid angle per unit energy interval, dE'dE` because E' is the energy of the outgoing neutron.

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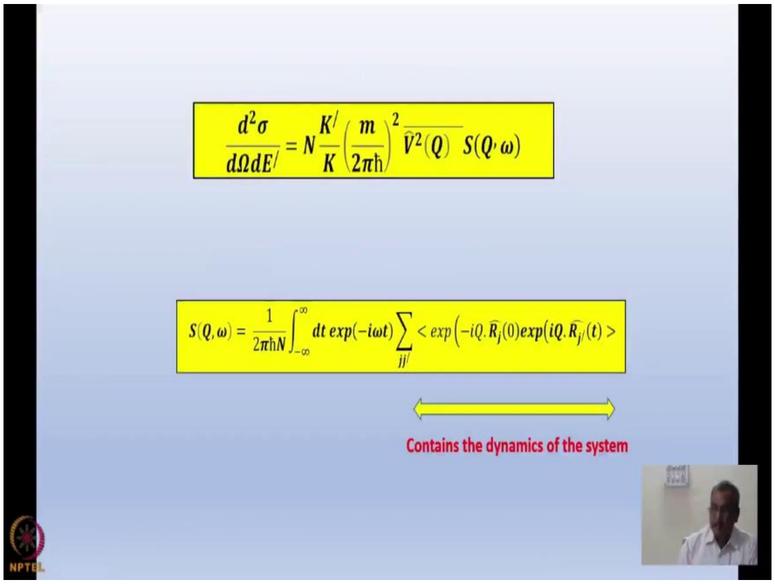

So, now, I can shorten the expression, I can write the scattering cross section as,

$$\frac{d^2\sigma}{d\Omega dE'} = N\frac{K'}{K}\left(\frac{m}{2\pi\hbar}\right)^2 \overline{\hat{V}^2(Q)} S(Q,\omega)$$

Here,

$$S(Q,\omega) = \frac{1}{2\pi\hbar N}\int_{-\infty}^{\infty} dt\, e^{-i\omega t} \sum_{jj'} \langle e^{-iQ.\widehat{R_j}(0)}\, e^{-iQ.\widehat{R_{j'}}(t)}\rangle$$

$\int_{-\infty}^{\infty} dt\, e^{-i\omega t} \sum_{jj'} \langle e^{-iQ.\widehat{R_j}(0)}\, e^{-iQ.\widehat{R_{j'}}(t)}\rangle$ is a Fourier transform of summation over all the sides jj` $\sum_{jj'} e^{-iQ.\widehat{R_j}(0)}\, e^{-iQ.\widehat{R_{j'}}(t)}$. I have given the signature of operators over here because in quantum mechanics these are supposed to be operators. But for all our calculations I can even take them as classical positions and it will not be too long when I do the derivation.

Now, right part contains the dynamics of the system and S(Q,ω) is in energy and Q space and over there when you took a Fourier transform over time I could go to S(Q,ω) in Q and ω space where I do the experiment. That means, I do my experiment where I find out the wavelength of the outgoing neutron at a certain angle and from there, I find out the energy change and the wave vector change and that experimental data is related to the dynamics of the system.