Statistical Mechanics
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Lecture - 44
Single Particle Quantum Partition Function Harmonic Oscillator – Part 1

Welcome back. So, we are interested in we looked at the density matrix for a free particle both in the momentum as well as in the coordinate presentation.

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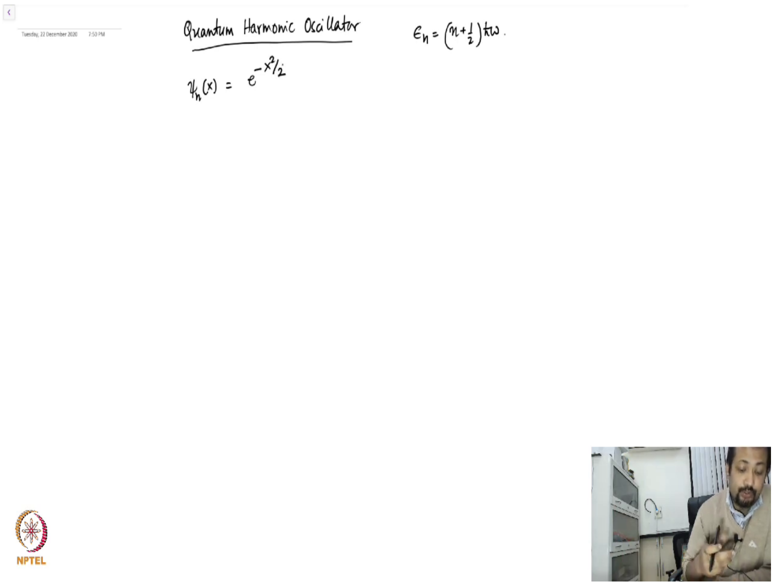

Now, we are interested in looking at the harmonic oscillator, single particle harmonic oscillator. So, I will write a Quantum Harmonic Oscillator. As you know that in this particular case the energy eigenvalues are discrete. So, I have n plus half h bar omega. And the energy eigen functions are given by e to the power minus x square over 2.

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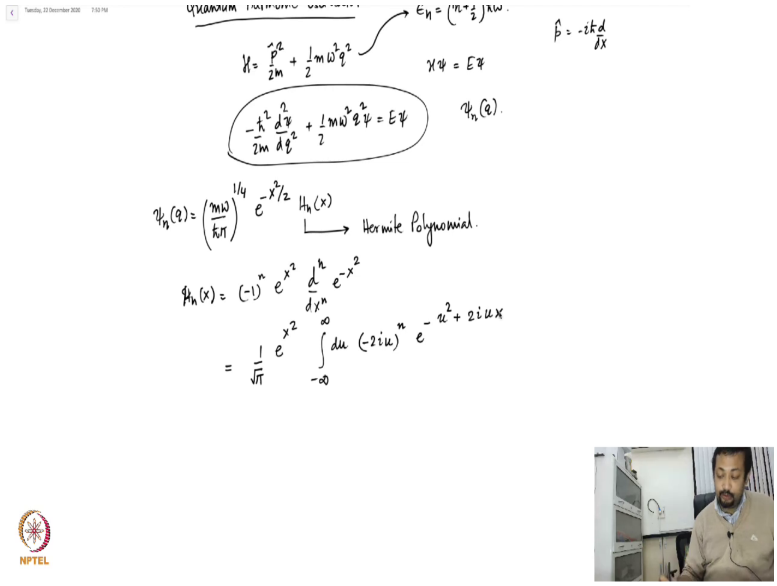

So, we will before we write this the Hamiltonian of the system is half p i p square over twice m plus half m omega square q square. This gives me discrete energy eigenvalue. Once I solve the equation as E of psi the operator p hat over here is ih bar d dx. So, that if I substitute this Hamiltonian, this becomes minus h square over twice m d 2 psi d x 2 plus half m omega square q square dq 2 because the coordinate in our case is q is going to be E times psi.

And we solve this equation to get the energy eigen functions psi n of q. And psi n of q is a little complicated is m omega h bar raised to the power one-fourth e to the power minus x square over 2, and then you have H n of x. This function is known as the Hermite polynomial, where H n of x is minus 1 raised to the power n e to the power x square d n dx n of e to the power minus x square.

So, once you operate the another derivative on this, finally, you are going to get a polynomial. Interestingly, this also has an integral representation and that is what we want to write down, we want to write down this as the integral presentation is square root pi e to the power x square minus infinity to plus infinity d u minus twice iu raised to the power n e to the power minus u square plus twice i v times x, sorry twice i u times x, because I am integrating over u there should not be any other variable.

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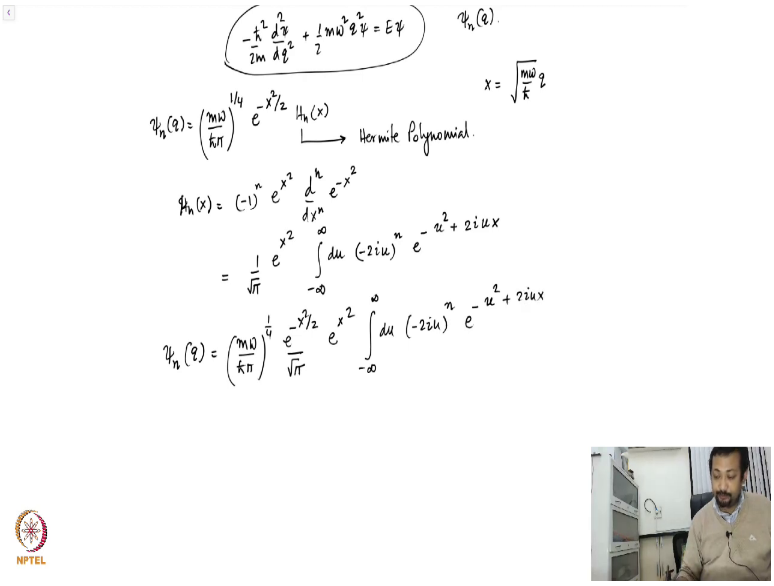

So, that psi by the way x here is square root m omega over h bar times q. So, psi n of q then becomes m omega h bar pi raised to the power one-fourth e to the power minus x square by 2 e to the power x square, square root of pi minus infinity to plus infinity du twice iu raised to the power n e to the power minus u square plus twice iux.

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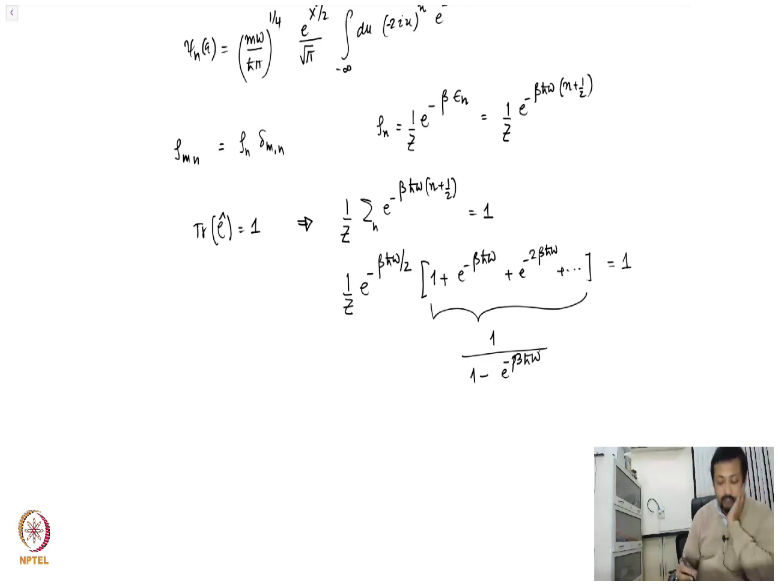

And this gives me m omega h bar pi raised to the power one-fourth e to the power x square by 2 square root pi minus infinity to plus infinity du twice minus of twice iu raised to the power n minus e to the power minus u square plus twice iux. We will later on use this relation.

Now, if you work in the energy basis, then of course your density matrix is very very simple rho mn is rho n delta of m, n, where rho n is going to be e to the power minus beta of epsa n 1 over Z, and you have 1 over Z e to the power minus beta h bar omega n plus half. If I now use that the trace of the density matrix must be 1.

This implies sum over n 1 by Z e to the power minus beta h bar omega n plus half is going to be 1, so that you have minus beta h bar omega 1 over Z. And if you open the sum, then you will see you are going to have a series and infinite series minus beta h bar 1 plus e to the power minus beta h bar omega twice beta h bar omega higher order terms is going to be 1. This is simply a geometric series whose sum is minus beta h bar omega.

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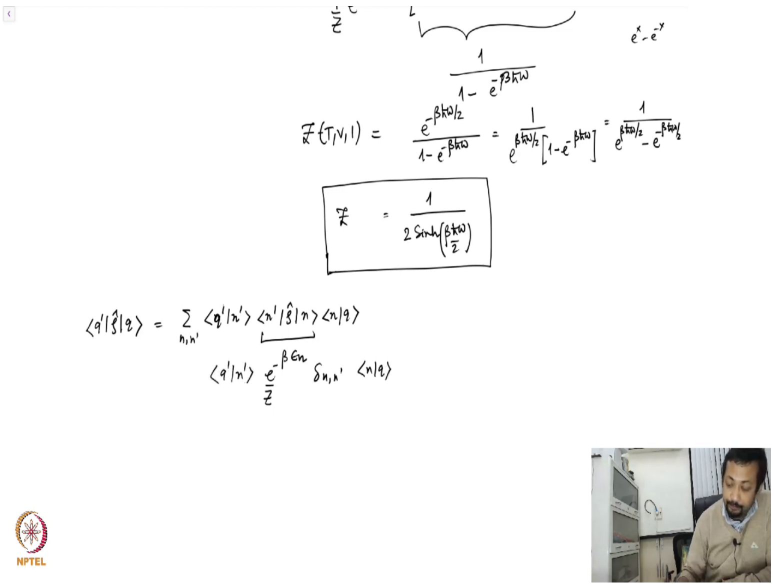

So, that the partition function T, V, 1 for a single harmonic oscillator is going to be minus beta h bar omega by 2 divided by 1 minus beta h bar omega. You can write down this as e to the power and beta h bar omega by 2 1 minus e to the power beta h bar omega which gives u 1 over e to the power beta h bar omega by 2 minus beta h bar omega by 2.

And this gives you we can immediately see that this as the form e to the power x minus x which is nothing but the sin hyperbolic function. So, you have an answer twice of sin hyperbolic beta h bar omega over 2. So, this is your partition function – micro-canonical partition function.

Now, the idea is to construct the density matrix in the coordinate representation. And this is where it becomes a little bit more involved, but it is very straightforward mathematics that is nothing extremely difficult which you cannot do. So, we write down this as n, n prime q prime n prime n prime rho hat n n of q. This quantity I know this is the density matrix in the energy presentation. And therefore, this becomes minus beta epsa n by Z delta n comma n prime and q q prime n prime.

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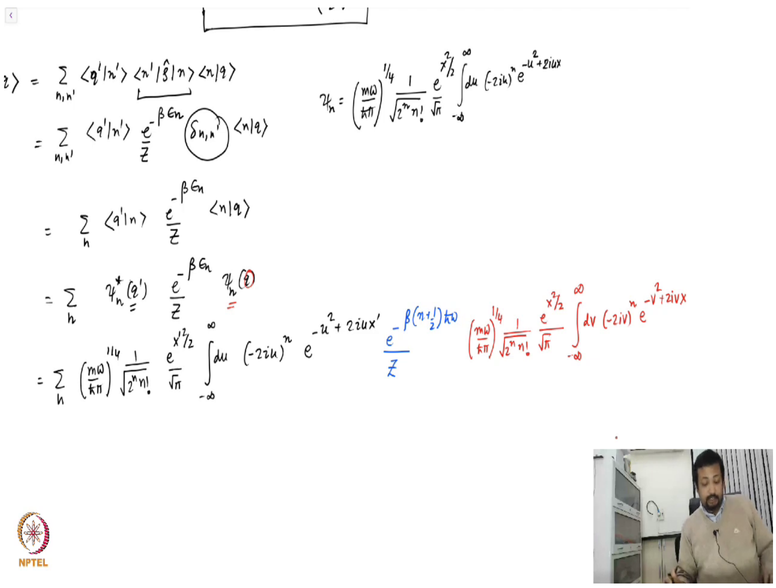

Now, clearly there is sum over n and n prime and I can carry forward I can take care of one of the sums over n prime to take care of this delta function, so that this becomes sum over n q prime n e to the power minus beta epsa n Z n of q. Let me see whether here I have missed out a factor that one should include. Where is that?

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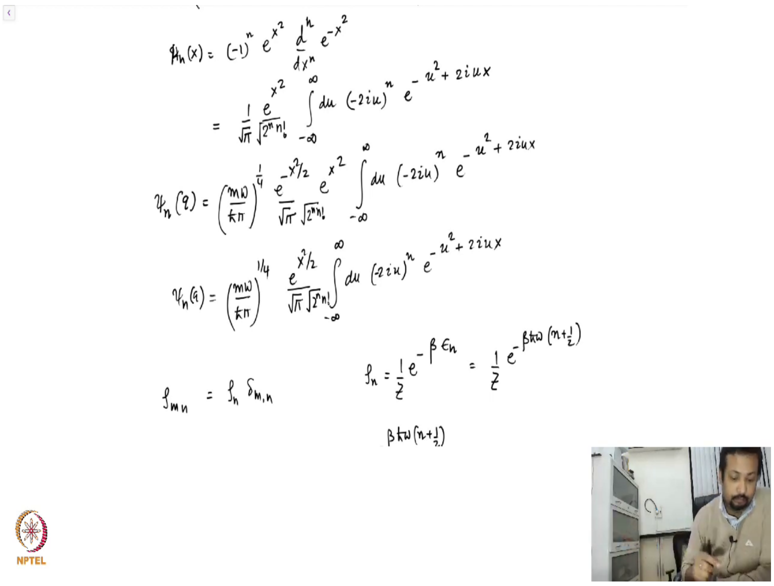

Yeah there has to be a 2 to the power n and n factorial with square root, there has to be a square 2 two to the power n, n factorial, square root 2 to the power n, n factorial this is the thing which I have missed not in h n x, but in psi n x not in h n x.

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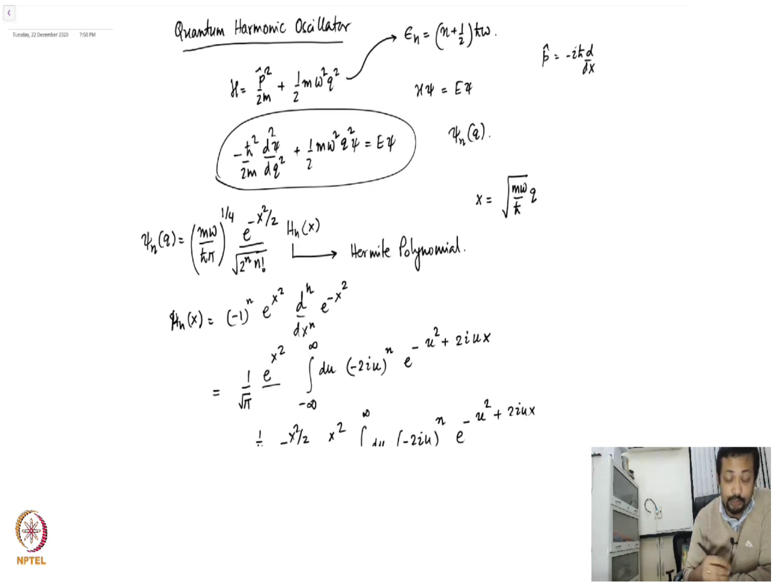

So, in psi n of q, yeah, here it has to be square root n factorial. And this comes from the normalization of this wave function right. So, this is sum over n this quantity is psi star n of q prime e to the power minus beta epsa n divided by Z, and this quantity is psi n of q. Such psi n of q as we have seen was m omega h bar pi 1 fourth square root 2 to the power n n factorial e to the power x square by 2 over square root pi.

And then I have this integral presentation of the Hermite polynomial which I use over here minus u square plus was there two factor, then yeah plus twice iu of x. So, then we write on this sum over n m omega over h bar pi one-fourth square root 2 to the power n, n factorial e to the power x prime square over 2 because this is q prime now. So, this becomes x prime square over 2 square root pi minus infinity to plus infinity du minus twice iu raised to the power n e to the power minus u square plus twice iux prime.

And then you have e to the power minus beta epsa n which is going to be n plus half h bar omega divided by Z, and then you have psi n of q which again gives you m omega over h bar pi raised to the power 1fourth 1 over square root 2 the power n, n factorial e to the power x square by 2, because this is now q not q prime square root of pi minus infinity to plus infinity dv minus twice iv raised to the power n e to the power minus v square plus twice ivx. I look horribly complicated.

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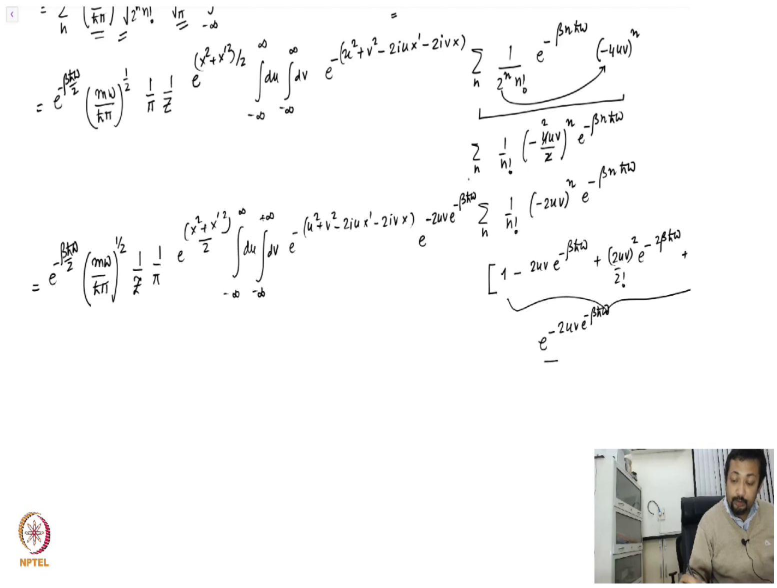

But things are going to simplify very soon. This together with this gives me m omega h bar pi half, then I have this square root pi and this square root pi that gives me 1 by pi, and I have a Z gives me 1 by Z right. The exponential factors that you see over here is not being integrated over neither is being sum.

So, it is x square plus x prime square by 2. Let us take the integrals over here du and then I have dv. Now, I take care of the sum n. But before that I also note that this factor that you see over here gives me eta e to the power minus beta h bar omega. So, I will bring out e to the power minus beta h bar omega. And hopefully, you have taken care of everything. Let us see.

Then I have this and this which is e to the power minus u square plus v square minus twice iux prime minus twice ivx times sum over n 1 over 2 to the power n, n factorial because you have a square root here and the square root here, the product of these two gives you 2 to be power n n factorial, and then you have e to the power minus beta n h bar omega; not only that now you also have this term and this term.

So, this term together that minus and minus gives you plus, 2, 2 gives you 4. But you have an i square, so that this is minus 4 uv raised to the power n. Let us concentrate on this sum, this sum I can write down as 1 over n factorial minus 4uv by 2. The 2 I can bring inside the bracket raised to the power n beta n h bar omega, which is sum over n 1 over n factorial the 2, 2 gets cancels out. And I have minus twice uv raised to the power n e to the power beta nh bar omega.

If you now write down this expand the whole thing, then the first term is 1, the second term is minus twice uv e to the power beta h bar omega, then you have twice uv whole square by 2 factorial e to the power twice beta h bar omega, and then we have higher order terms. And if you look at this carefully, then you see that this is nothing but the expansion of minus twice uv e to the power minus beta h bar omega.

So that what you originally started off with now reduces to beta h bar omega m omega over h bar pi half 1 over Z and 1 over pi, then you have x square plus x prime square by 2 you have minus infinity to plus infinity du minus infinity to plus infinity dv you have e to the power minus u square plus v square minus twice iu x prime minus twice ivx, and then you have this which is e to the power minus 2 uv e to the power minus beta h bar omega.

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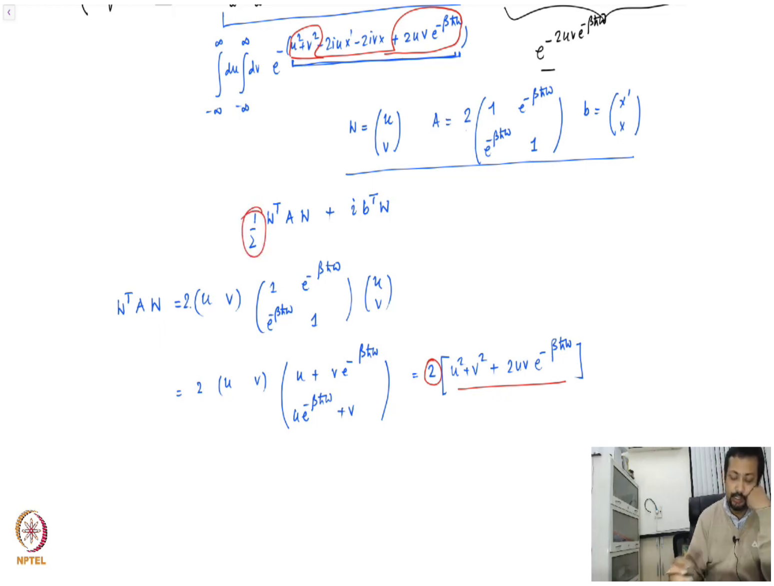

Now, we concentrate on this integral. So, we will rewrite this integral as du infinity dv e to the power minus u square plus v square minus twice iu x prime minus twice ivx. And then I have 2uv e to the minus beta h bar omega. This happens to be a multivariate Gaussian integral. This term that you see over here I can write down this as half of b transpose A, sorry not b transpose w transpose.

Now, to evaluate this, you define a vector a column vector which is going to be your u and v, a matrix A which is going to be your 1 e to the power minus beta h bar omega e to the power minus beta h bar omega 1, and another column vector which is going to be your x prime x. Once you have defined this you can recurs this part that is underlined over here as half of W transpose A W plus i b transpose W which is basically b dot W.

W transpose A W is going to give you u v 2 times this, the 2 comes from this part 1 e to the power minus beta h bar omega e to the power minus beta h bar omega 1 times u v. So, that if you now do this, this is going to be twice u v times u plus v e to the power minus beta h bar omega u e to the power minus beta h bar omega plus v.

And if you multiply now this one – the transpose, you are going to get u square plus v square plus twice uv minus beta h bar omega. So, that you see u square plus v square combined with this is given by this term. The two factor that you see cancels with this half factor.

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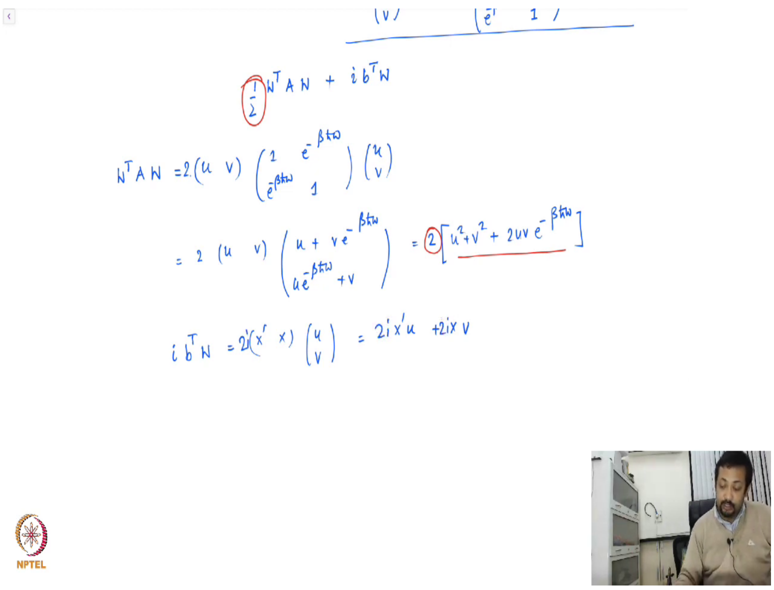

Similarly, b transpose W is going to be x prime x u v which is going to be x prime u plus xv. And b transpose has to be ok, so b there has to be a factor 2 here. So, i times b transpose is going to be 2 i, and I have 2 i; and I have 2 i and that is precisely what I have.