Statistical Mechanics
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Lecture - 45
Single Particle Quantum Partition Function Harmonic Oscillator – Part II

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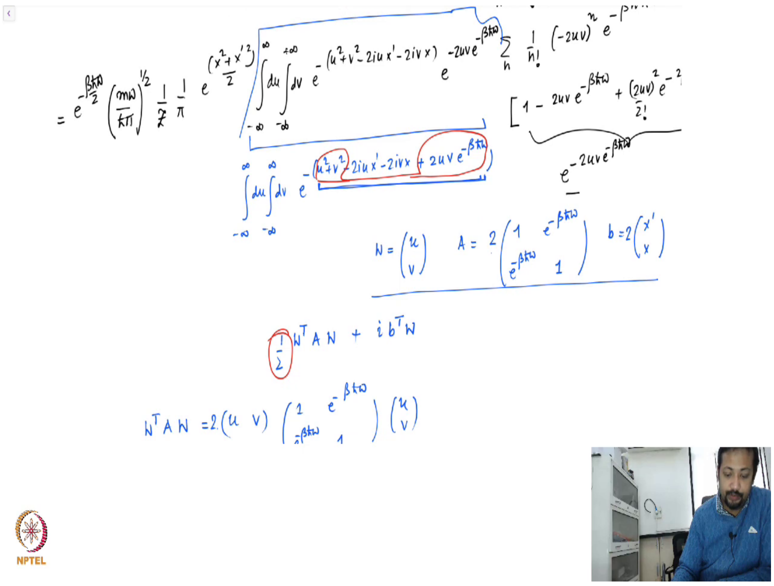

So now, we want to look at this integral. Now, as we said that this is a multi dimensional Gaussian integral. How do we evaluate that? It is not very complicated, it is very very simple.

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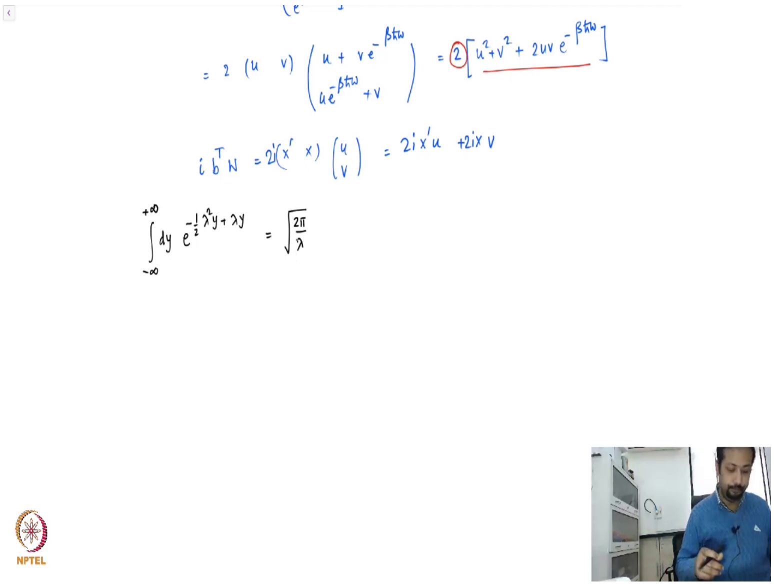

So I know, that we start off from this that minus infinity to plus infinity d y e to the power, so e to the power lambda square half lambda square y minus plus lambda y is just going to be square root 2 pi over lambda [FL].

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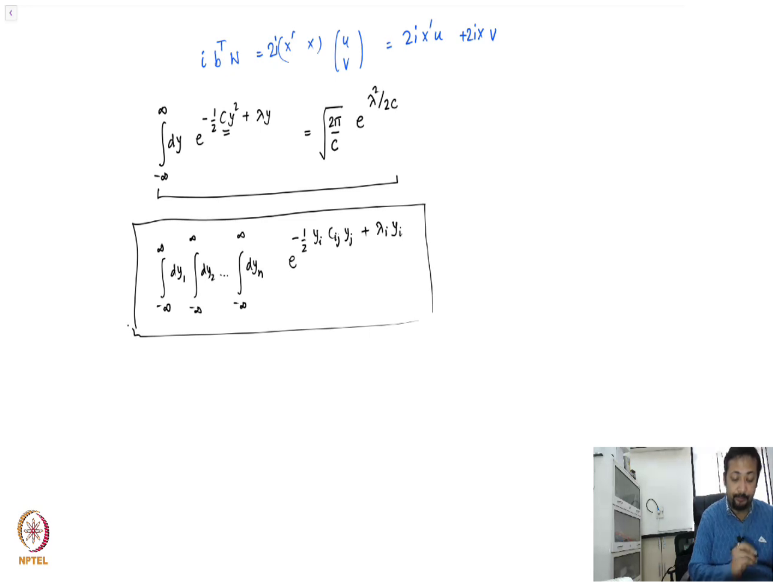

So, we start off from the integral minus infinity to plus infinity d y minus half C y square plus lambda y and this integral is a standard Gaussian integral and the answer to that is 2 pi over C e to the power lambda square over 2 C. The general multi dimensional case, generalization of this integral is minus infinity to plus infinity d y 1 minus infinity to plus infinity d y 2 so on and so forth. You have d y n.

So now, you have n Cosh variables and this particular term becomes minus half y i C i j y j plus lambda i y i.

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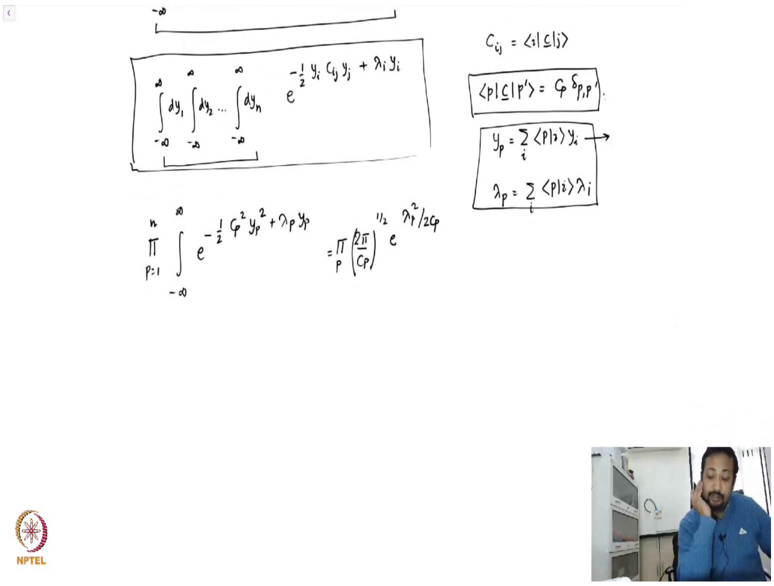

So, this is the integral that we are interested in evaluating. For this I have the matrix C i j which is given by i C j. Now, I can diagonalize this matrix and determine the orthonormal Eigen functions, so that p C p bar prime becomes C p delta p p prime. So, I go from this representation of i to this which are also orthonormal, so that my matrix C becomes a diagonal matrix.

And in which case you have y p is going to be sum over i p i y i and lambda p is going to be sum over i p i lambda i. The Jacobian of this transformation is unity that one should take care I mean that is obvious you can use this relation to determine the Jacobian of this matrix and your integral now this whole part becomes product over p is equal to 1 to n minus infinity to plus infinity e to the power minus half C p square y p square plus lambda p y p.

Which is going to be 2 pi C p product over p raised to the power half e to the power lambda p square over 2 C p. This is a very elegant and simple answer and once you use these relations carefully then you will see.

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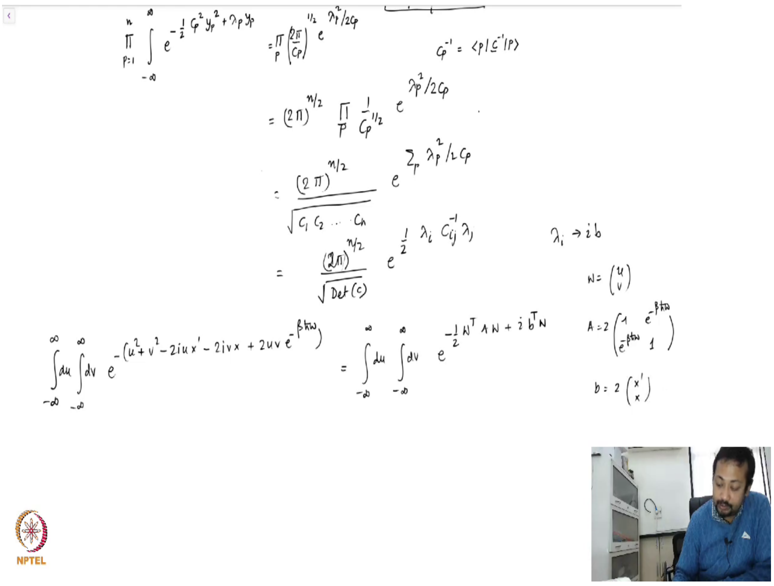

So, this quantity now becomes 2 pi raise to the power n by 2 since y i runs from y i equal to 1 to n. And then, you have a product over p 1 over C p raised to the power half e to the power lambda p square over 2 of C p. This you can further simplify as 2 pi raised to the power n by 2 square root of C 1 C 2 C n e to the power sum of a p lambda p square over 2 C p.

If you use this relations over here, these have been highlighted over here, then you see, first of all you identify that the denominator is going to be 2 pi raised to the power n by 2 divided by square root of determinant of C. And this quantity is going to be half comes out lambda i C inverse i j lambda j. But note that we have lambda i as i times b.

So, in our case we will have a factor minus (Refer Time: 6:25), but we will not worry about that when we actually write down that integral. So, we have to now evaluate minus infinity to plus infinity d u minus infinity to plus infinity d v e to the power minus u square plus v square minus 2 i u x prime minus 2 i v x plus 2 u v e to the power minus beta h bar omega.

And this we said, I can write down this as minus infinity to plus infinity d u minus infinity to plus infinity d v e to the power minus half v sorry W transpose A W plus i b transpose times W, where we had written down the matrix W was u v A was 2 1 e to the power minus 2 sorry e to the power minus beta h bar omega e to the power minus beta h bar omega 1 and b was 2 x prime and x.

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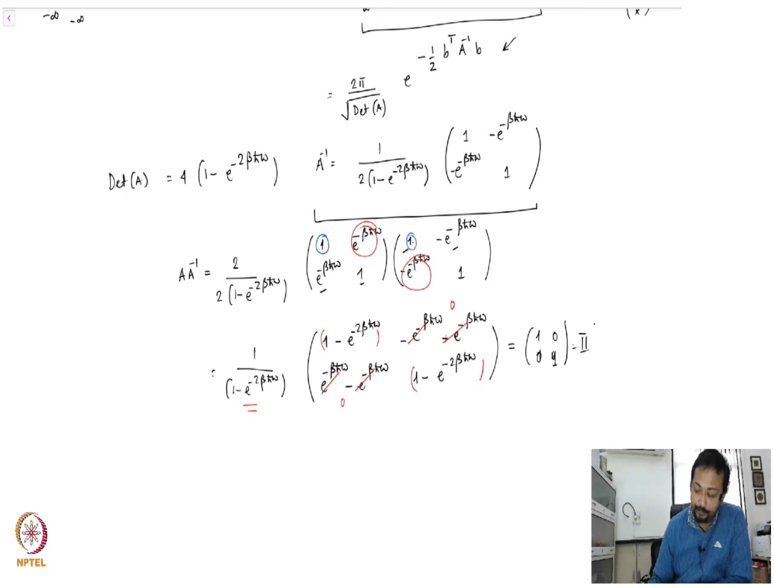

The answer follows from this. This is going to be n is equal to 2 in our case. So, we will have 2 pi divided by square root of determinant of A e to the power minus half, minus comes in because you we identify lambda i as i times b. So, where this is going to be b transpose A inverse b. Let us take it step by step determinant of A follows from this relation is going to be 4 1 minus e to the power minus 2 beta h bar omega.

Please make sure that the factor is 4 outside and not 2 blindly, because 2 multiplies all the elements of this matrix A. And then A inverse is evaluated as half 1 minus e to the power minus 2 beta h bar omega. And you will have 1 and 1 you will have minus e to the power minus beta h bar omega and you will have minus e to the power minus beta h bar omega. So note that this diagonalization that we did, we wrote down this result in this particular form because it is a symmetric matrix invertible matrix.

If you have any doubt about this, one can easily verify that A A inverse is going to be 2 times 2 1 minus 2 beta h bar omega, and then I have A as 1 e to the power minus beta h bar omega e to the power minus beta h bar omega 1 and the inverse is 1 e to the power minus beta h bar omega minus e to the power minus beta h bar omega 1.

So, that this is going to be, let us cancel out the 2's and write them as 1 over 1 minus 2 beta h bar omega. This time the first element is going to be 1 minus 2 beta h bar omega this multiplies this, so this multiplies this and this multiplies, this for the first element. The second element is going to be minus e to the power minus beta h bar omega plus e to the power minus beta h bar omega.

This element is going to be e to the power minus beta h bar omega. This multiplies this and then 1 multiplies this gives you minus beta h bar omega. Finally, the last element is going to be 1 minus 2 beta h bar omega. So, things cancel out, this this cancels out to give you 0, this one this one cancels out to give you 0, and you see this factor and this factor cancels out with the pre factor that is outside to give you the identity matrix 1 0 0 1 which is i. So, indeed our A inverse works nicely, good.

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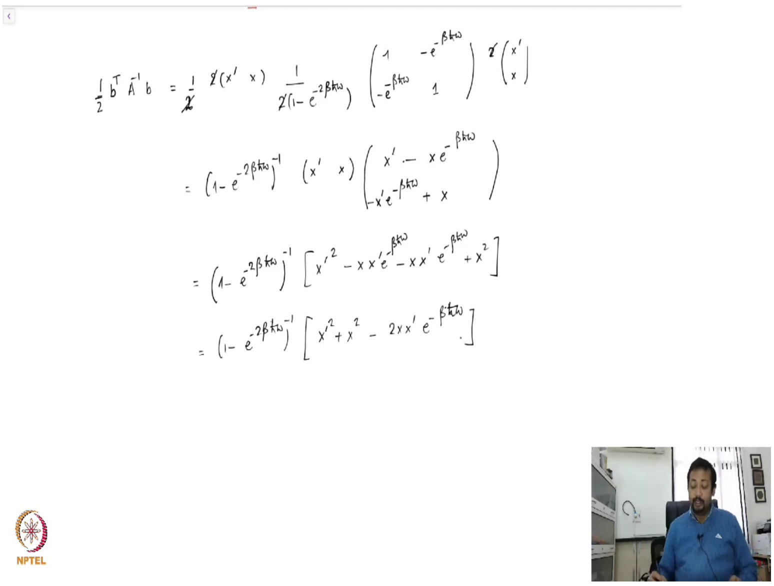

So, all I have to figure out now is what is half b transpose A inverse b which is going to be half b transpose is 2 x prime x and then I have a half that this factor in A inverse I have 1 minus e to the power minus beta h bar omega minus beta h bar omega 1 and then I have 2 again the factor at b.

So, these 2 cancels with these 2, this 2 cancels with this 2 and I have 1 minus e to the power minus 2 beta h bar omega inverse x the b transpose and if I do the matrix multiplication I will have x prime minus x e to the power minus beta h bar omega and then I am going to have minus x prime e to the power minus beta h bar omega plus x.

So that, this becomes 1 minus 2 beta h bar omega inverse and I have x prime square minus x x prime minus x x prime sorry e to the power minus beta h bar omega should be here, e to the power minus beta h bar omega should be here, and then I am going to have x square. Looks very nice and elegant and I can write down this as 1 minus 2 beta h bar of omega inverse x prime square plus x square minus 2 x x prime e to the power minus beta h bar of omega.

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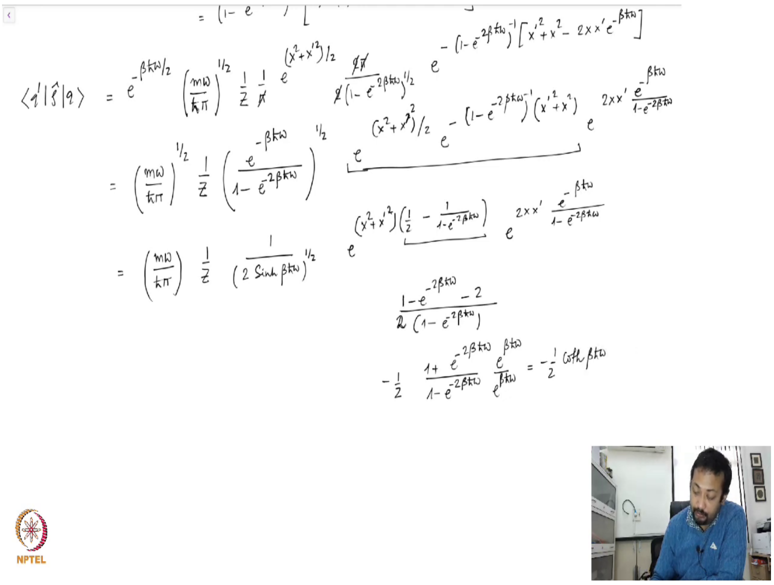

Let us go back to the representation we were writing. The coordinate representation of this and write all the terms we will see then where further simplification is required. Half and then I have 1 of a set 1 over pi, there is a 2 pi which sorry before that before this integral there is also the factor e to the power x square plus x prime square by 2.

And then I have the integral the 2 dimensional Gaussian integral which gives me 2 pi, the determinant of C square root of that which will give me 2 1 minus e to the power minus 2 beta h bar omega half and then I will have e to the power minus of half b transpose A inverse b, which is going to be e to the power minus 1 minus 2 beta h bar omega inverse times x prime square plus x square minus 2 x x prime e to the power minus beta h bar of omega. So you are almost done.

So, this is going to be m omega over h bar times pi raised to the power half. Now, this pi this pi cancels this 2 this 2 cancels, therefore nothing I have to worry about, I have 1 over Z and then this is e to the power minus beta h bar omega 1 minus e to the power minus 2 beta h bar omega raised to the power half. I have then e to the power x square plus x prime square by 2 e to the power minus 1 minus e to the power minus 2 beta h bar omega inverse.

And I have x prime square plus x square times e to the power 3 x x prime e to the power minus beta h bar omega 1 minus 2 beta h bar omega. It is a bit of a tedious algebra. It is a little bit complicated, but its a good exercise to do for once at least in your lifetime. So, this is going to be m omega over h pi 1 over z, let us see what this gives me. This gives me 1 over 2 sin hyperbolic beta h bar omega raised to the power half.

And then, let us first combine these two pre factors. Once you combine these two pre factors, I have e to the power x square plus x prime square half minus 1 over 1 minus 2 beta h bar omega and then I have 2 x x prime e to the power minus beta h bar omega 1 minus e to the power minus 2 beta h bar omega.

This factor is half 1 minus 2 beta h bar omega minus 2 divided by 1 minus 2 beta h bar omega. The simplification gives you minus half 1 plus e to the power minus 2 beta h bar omega divided by 1 minus 2 beta h bar omega, which you immediately see, I can multiply this by e to the power, I can multiply the numerator as well as the denominator by beta h bar omega and this gives me minus half Coth hyperbolic beta h bar omega.

The coefficient of this is going to be 2 x x prime, we will keep it like this e to the power beta h bar omega minus e to the power beta h bar omega. In fact, this is just going to be sin hyperbolic.

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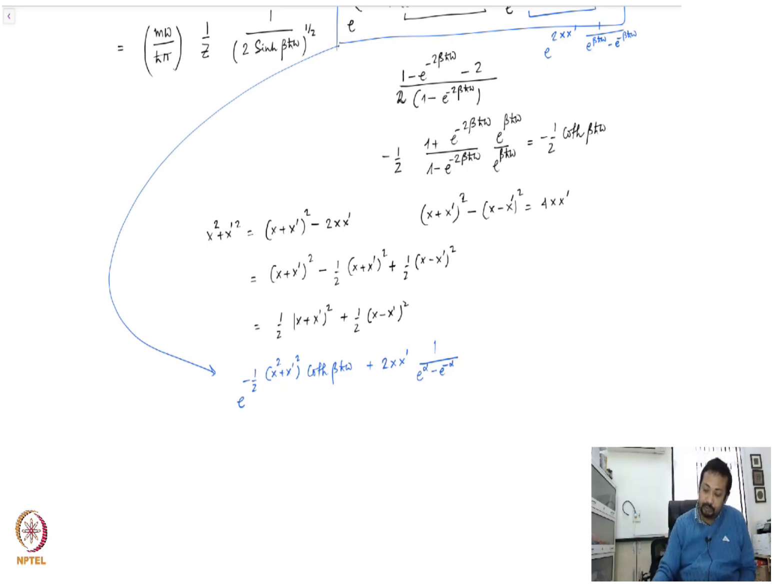

The goal is, now well, we can write down x square plus x prime square as x plus x prime whole square minus 2 x x prime. And we also know that x plus x prime whole square minus x minus x prime whole square sorry plus is going to be 4 x x prime. So that, this I can now replace as x plus x prime whole square minus half of x plus x prime whole square plus half of this is going to be minus, you know I think this is wrong this relation is wrong.

So, this has to be minus, so that this becomes a plus is going to be x minus x prime whole square. And therefore, you have half of x plus x prime whole square plus half of x minus x prime whole square. So that the exponential part that we have over here, let us write them down like this way, is going to be e to the power minus half x plus x prime whole x square plus x prime square Coth hyperbolic beta h bar omega, and then I have plus 2 x x prime 1 over e to the power alpha minus e to the power minus alpha.

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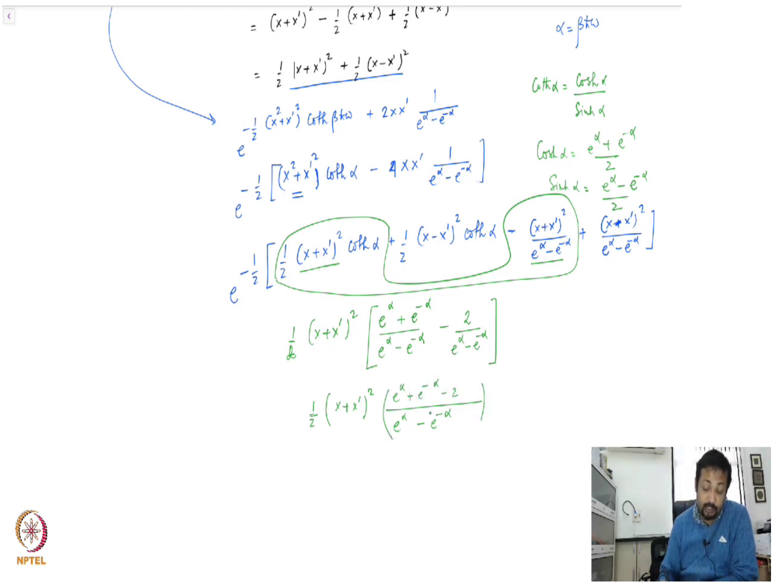

Which we will write down as minus half x square x prime square Coth hyperbolic alpha, where we have identified alpha as beta h bar omega plus 2, this has to be 4 x and x prime 1 over e to the power minus of all 1 over e to the power alpha to the power minus alpha. In fact, life becomes very simple if you write down this in terms of sign hyperbolic alpha, but in this case the calculation becomes more explicitly clear.

So, let us write down substitute this one over here, this becomes half x plus x prime whole square Coth alpha plus half x minus x prime whole square Coth alpha 4 x x prime is this has to be minus this has to be minus because I have taken a minus outside common.

So, this becomes minus x plus x prime whole square over e to the power alpha minus alpha minus and this becomes plus x plus x x minus x prime whole square e to the power alpha minus e to the power minus alpha. So, of course, you have e to the power minus half outside looks a very complicated expression, but it is going to simplify very nicely. Let us take this term and this term together.

So, I will take this term and this term and group them together. So, that I have half of x plus x prime whole square Coth hyperbolic alpha is e to the power alpha plus e to the power minus alpha divided by e to the power alpha minus e to the power minus alpha minus 2 over e to the power alpha e to the power minus alpha.

So, if you are unfamiliar with the hyperbolic function, this is going to be Cosh alpha over sin hyperbolic alpha Cosh alpha is e to the power alpha e to the power minus alpha by 2 and sin hyperbolic alpha is going to be e to the power alpha e to the power minus alpha by 2. So, that this gives me half x plus x prime whole square e to the power alpha minus e to the power minus alpha and I have e to the power plus alpha minus alpha minus 2.

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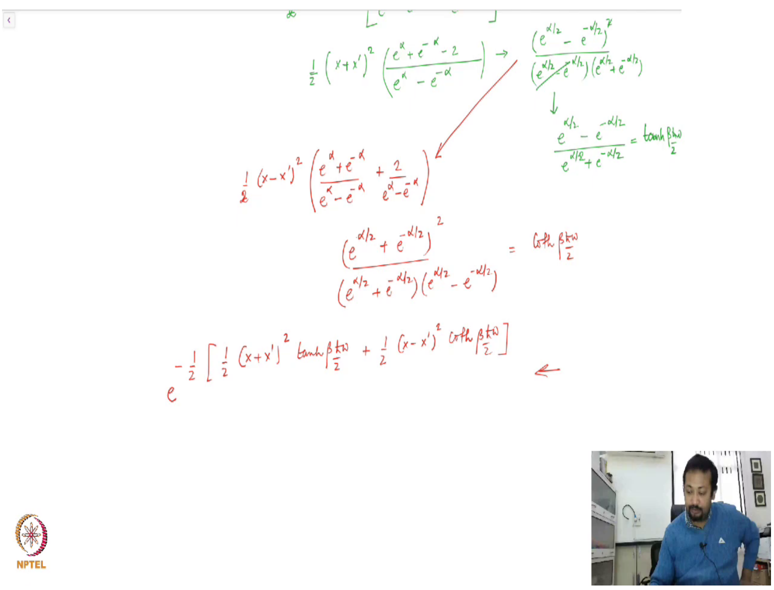

Now, this expression if you follow it carefully, you see the denominator is like a square minus b square, which I can write down the denominator as e to the power alpha by 2 minus e to the power minus alpha by 2 and then e to the power alpha by 2 e to the power minus alpha by 2 the numerator is you see very nicely alpha by 2 minus minus alpha by 2 whole square.

So, that this term is now e to the power alpha by 2 minus e to the power minus alpha by 2 divided by e to the power alpha by 2 plus e to the power minus alpha by 2. Because one factor cancels with this one and this quantity is tan hyperbolic beta h bar omega by 2.

So, similarly if you now look at this term and combine it with this term you are going to get half of x minus x prime whole square. Coth hyperbolic alpha is again e to the power alpha plus e to the power minus alpha divided by e to the power alpha minus alpha minus 2, sorry this has to be plus now, both of them have the plus signs e to the power alpha e to the power minus alpha.

Again one follows it the same root like this and one comes up with e to the power alpha by 2 plus e to the power minus alpha by 2 whole square divided by e to the power alpha by 2 plus e to the power minus alpha by 2 times e to the power alpha by 2 minus e to the power minus alpha by 2.

And this you immediately see is going to be Coth hyperbolic beta h bar omega by 2. So, your expression for the exponential then reduces to minus half half x plus x prime whole square, it is a very elegant expression, tan hyperbolic beta h bar omega by 2 plus half x minus x prime whole square Coth hyperbolic beta h bar omega by 2. And this is the term we will keep it in our record in our memory.

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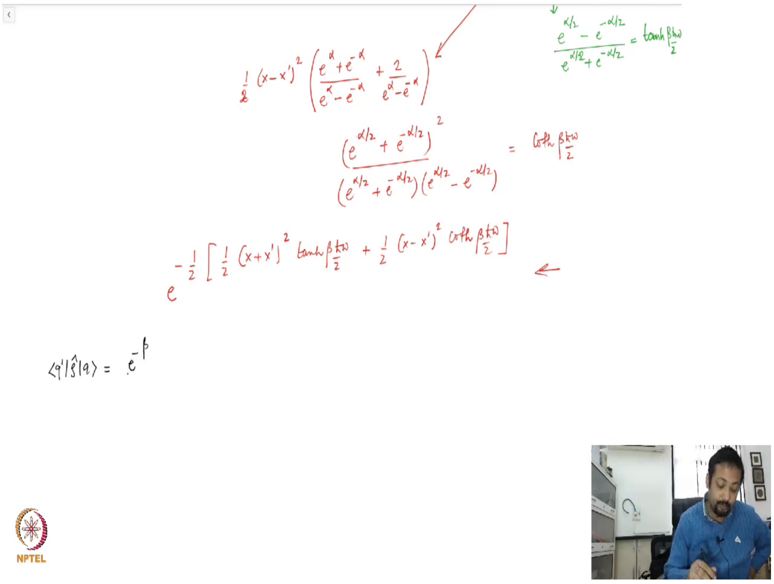

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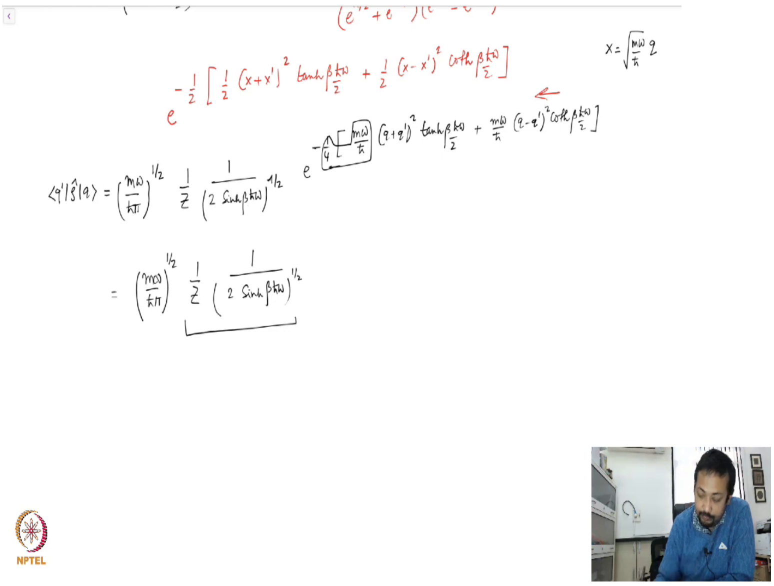

And then, we have q prime rho hat cube as e to the power minus sorry e to the power minus beta h power omega was already taken care of, we have m omega over h bar pi raised to the power half 1 over Z and then we have 1 over 2 sine hyperbolic beta h bar omega raised to the power half.

Am I right? Correct. And then I have e to the power half factor I can bring out the exponential is going to give me minus one-fourth x was square root m omega over h bar times q. So, that x prime becomes m omega over h bar q plus q prime whole square tan hyperbolic beta h power omega by 2 plus m omega over h bar q minus q prime whole square Coth hyperbolic beta h bar omega by 2.

So that, I have m omega over h bar pi raised to the power half 1 over set 1 over 2 sine hyperbolic beta h bar omega half.

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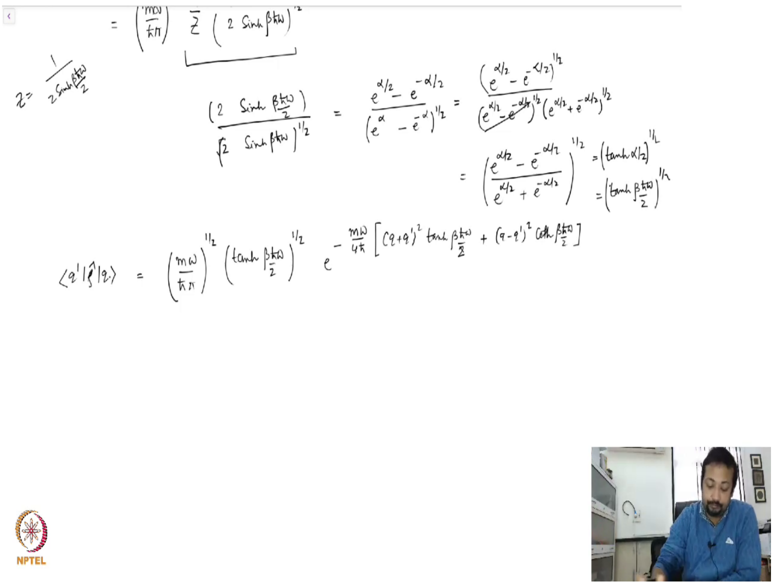

So, let us see if we can simplify this. If I just look at this term, this is going to be 2 sine hyperbolic beta h bar omega since I know that Z is 1 over 2 sine hyperbolic beta h bar omega for the single particle which we have already calculated. This becomes square root of 2 sine hyperbolic beta h bar omega, let us just say half. This I simplify as e to the power alpha minus e to the power minus alpha, and this as e to the power alpha by 2 minus e to the power minus alpha by 2.

Sorry, I think there is a mistake here, this is going to be half this is going to be half. So, that this is half this is half and the other one does not contain the half factor. And this is raised to the power half. This simplifies to minus alpha by 2 divided by e to the power alpha by 2 minus e to the power minus alpha by 2 raised to the power half times e to the power alpha by 2 e to the power minus alpha by 2 raised to the power half.

This factor gives you a half in the numerator and you have e to the power alpha by 2 minus e to the power minus alpha by 2 divided by e to the power alpha by 2 plus e to the power minus alpha by 2 whole raised to the power half, and this answer you know is tan hyperbolic alpha by 2 which is tan hyperbolic beta h bar omega by 2.

So that this becomes m omega over h bar times pi raised to the power half and then this raised to the power half do not forget that. I have tan hyperbolic beta h bar omega by 2 raised to the power half. The exponential factor becomes m omega over 4 h bar times q plus q prime whole square tan hyperbolic beta h bar omega by a 2 plus q minus q prime whole square Coth hyperbolic beta h bar omega by 2.

And this is the expression that you are looking for it is complicated, but nevertheless we have got where we wanted to come. We have reached where we wanted to reach.

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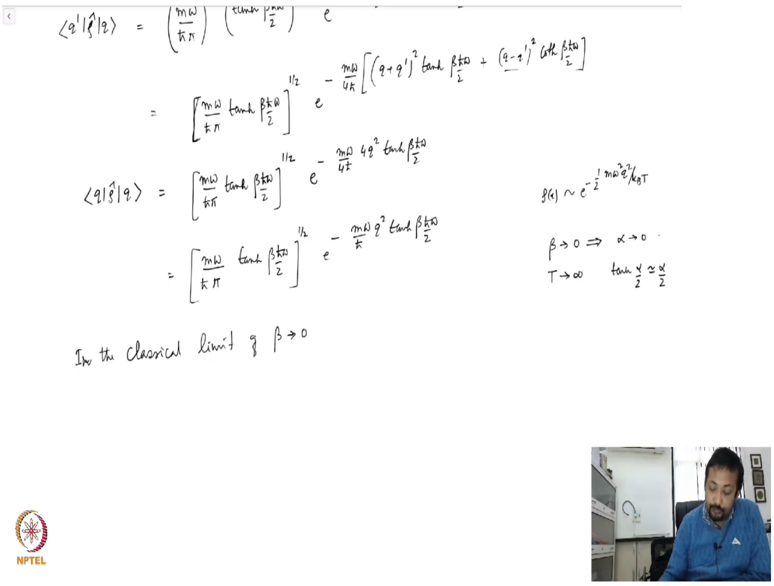

A little simplification would give me m omega over h bar pi tan hyperbolic beta h bar omega by 2 raised to the power half is e to the power minus m times e to the power minus m omega over 4 h bar q plus q prime whole square. Tan hyperbolic beta h bar omega by 2 plus q minus q prime whole square Coth hyperbolic beta h bar omega by 2.

Now I want to test. So, I know that for the particle to be in the queue it is the diagonal elements essentially represents that the particle is in the given state. So, if I evaluate q rho hat q and in the classical counter part of this is rho of q, we have seen this for the ideal gas, I mean a single particle free particle where this corresponded to 1 by V.

Here, this corresponds to m omega over h bar times pi, and then I have tan hyperbolic beta h bar omega raised to the power half e to the power minus m omega over 4 h bar q is q prime, so this gives me 4 q square tan hyperbolic beta h bar omega by 2 and this term vanishes.

So that I have m omega over h bar times pi tan hyperbolic beta h bar omega by 2 raised to the power half e to the power minus, I will have m omega over h bar times q square tan hyperbolic beta h bar omega by 2. Now what do I expect in the classical limit? If I go take this system in the classical limit, I would expect that it will have a canonical distribution. So, which means that rho of q must go as e to the power minus half m omega square q square over K B T.

So therefore, let us look for the case when beta tends to 0, the approximation and which means T tends to infinity and therefore, this implies beta tends to 0 means alpha tends to 0, because I have beta h bar omega. So, tan hyperbolic alpha is approximately alpha and therefore, tan hyperbolic alpha by 2 is also approximately alpha by 2. So that in the classical limit of beta going to 0.

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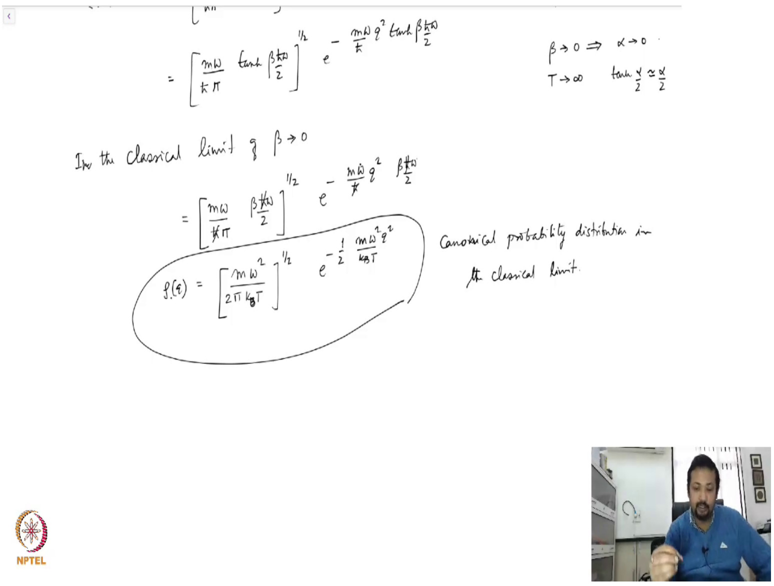

This becomes m omega over h bar times pi and then I have beta h bar omega over 2 raised to the power half e to the power minus m omega over h bar q square beta h bar omega by 2, h bar h bar cancels out and then I have m omega square over 2 pi K B T. This is becoming a little bit of a tricky issue. Now, K B T raised to the power half and then you have the half factor comes over here the h bar h bar cancels, I have omega and omega gives me omega square m omega square q square, I have a beta which is K B T.

So, you see this result is exactly the canonical probability distribution in the classical limit. So, in fact we have come up with the correct expression and this corresponds to rho of q.