Statistical Mechanics
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Lecture - 35
Problem solving demo - part 1

So, good afternoon students, this is the last lecture of our course. And today, we will continue with the problem solving that we started off in the last meeting. So, today I am going to talk about some correlation function that you can compute for the system of fermions in quantum; is quantum systems. So, one would like to know, how we deal with fluctuations of occupation numbers in a gas of fermions for example. So, let us recall a few things.

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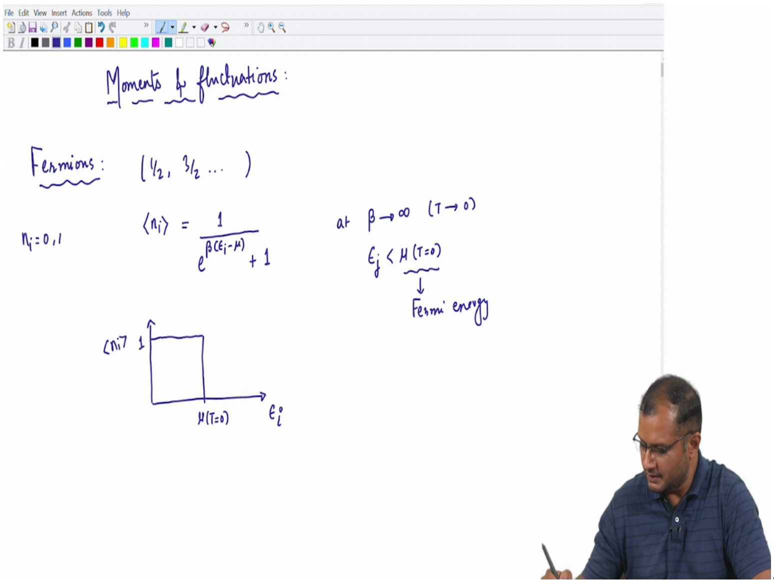

So, we will talk about simple correlations and I would rather call them as moments and fluctuations; and these moments and fluctuations can be very easily used to construct correlations of the occupation number. So, I will start with the simple case and you can extend this to the case of bosons as well. So, the fermions if you recall these are systems with half a dangerous spins and we know that their statistics follow the Fermi Dirac rules.

So, if you recall the average occupation number of any level i; i here is a single particle state and if I am interested in the average occupation number. We know that n i can be 0 and 1 for Fermions, but the average n i is not 0 or 1. So, this is computed as 1 over e to the power beta E i minus mu plus 1.

So, as you can tell that at 0 temperature or 0 Kelvin when, beta goes to infinity for any energy level which is less than the chemical potential at t equal to 0 and chemical potential at t equal to 0 is nothing but the Fermi energy, the occupation number is 1; the average occupation number is 1. So, if I compute, if I sketch this occupation number at t equal to 0; I would get something like this. So, there would be somewhere a chemical potential at t equal to 0, this is a value on the x axis; this is also the Fermi energy. And everything below this Fermi energy would be occupied as 1 and this is where the graph would abruptly come to 0 ok.

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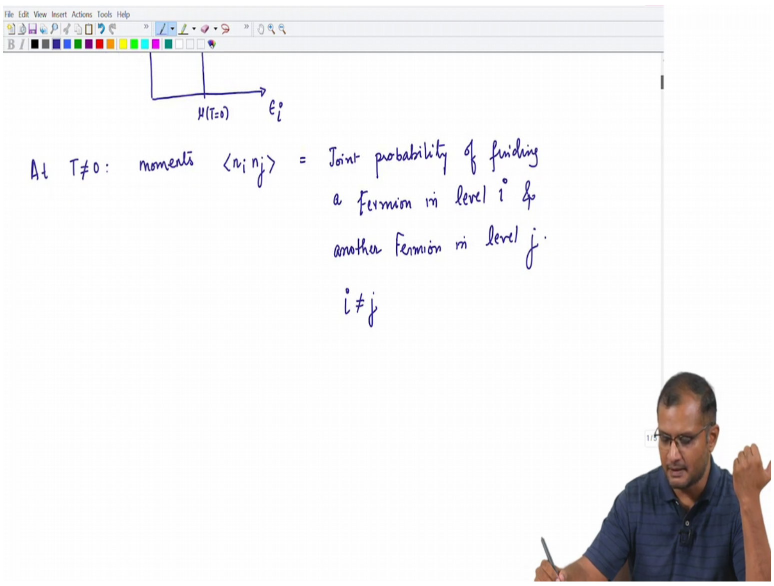

So, if you are interested in for example, at finite temperature if you want to compute some correlation or moments of the occupation number. Then, we would be computing variables such as; we will computing functions such as these moments and I would like to just highlight why these moments are useful here. So, for example, you can be; you may be interested in computing the joint probability density of finding of fermion in level i and another fermion. So, this joint moment n i n j is a joint probability of finding a fermion in the single particle level i and another fermion in the level j, we have taken this convenient assumption that i is not equal to j ok.

So, we are talking about different single particle levels and we are talking about the probability of finding one fermion in level i and some other fermion in level j ok. And this can be computed; so, this is a relevant question and this can be computed by this joint moment ni nj. So, moments are important here ok, they give a some physical picture you know of something or some importance ok.

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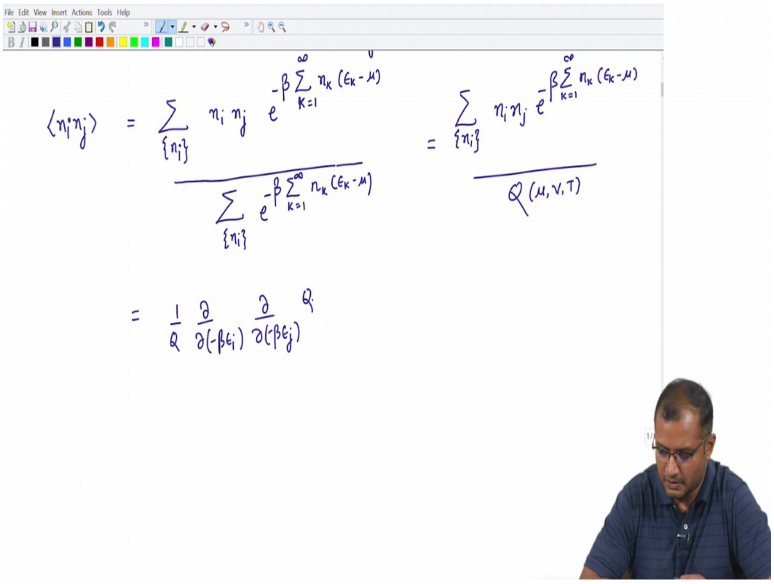

So, immediately I know that the joint moment is important and so we would like to compute that. So, let us compute this joint moment ok. So, if you recall this joint moment is nothing but the expectation value of n i n j; so, these are two variables ni and nj. And suppose, I sum over all possible microstates and sample the n i n j ok, this is the variable whose average is required, in the distribution which is given as e to the power; so, this is my probability distribution.

Some, I will take a different variable here. Let us say K, which goes from 1 to infinity n K E K minus mu ok. So, here this variable will go from 1 to infinity because we have finite energy levels right. And naturally, this has to be divided by the norm which is the, which is our familiar partition function. So, I am going to write down once explicitly, but very soon I will be writing it with symbol.

So, this is basically where, this entire denominator is basically the grand canonical partition function ok. So, this is like; let us write this once more, n i sorry I have just made a small mistake here. So, this is summation over all the possible microstates; set of n is ok that is my microstate, my variable n i n j, the product of two random variables E to the power minus beta divide by my grand partition function ok.

So, you can see that this can be written as; if you look at the numerator, this looks like the derivative of my partition function with respect to the variable n j and n i. So, this is like a twice derivative of the partition function so, this is like 1 upon Q ok.

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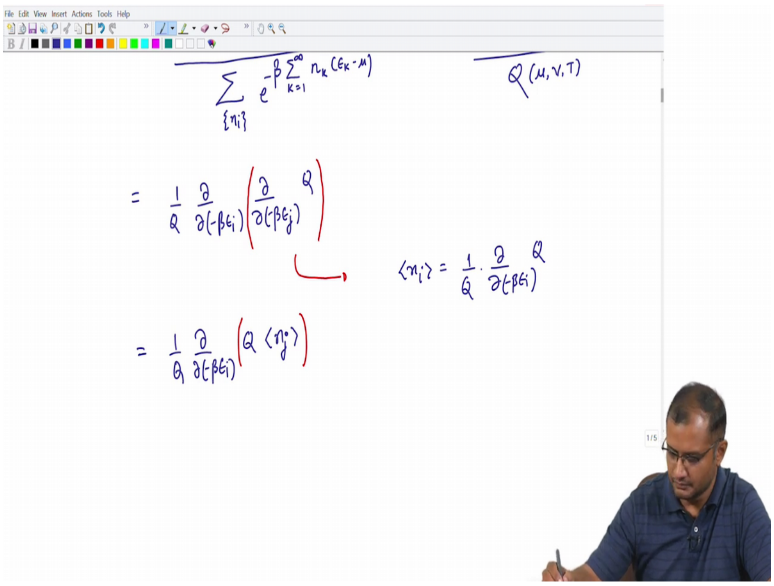

So, the innermost derivative can be easily replaced by something that you already know ok. So, let us replace the innermost derivative as; so, by the definition of average occupation number. This is nothing but; so, I know already that my average occupation number which is n i is given as 1 over Q d over ok.

So, which means the bracketed object in under red bracket is nothing but Q times nj, average occupation number of the j th single particle level q times; so, this is the bracketed thing. So, let me remove the; so, that we know that the red bracket is replaced by a new red bracket ok; so, sort of homogeneity alright.

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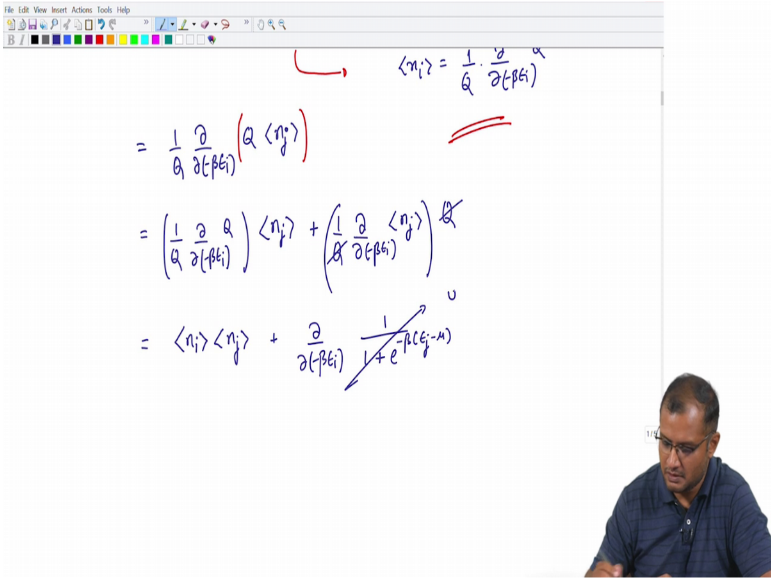

So, now this basically simplifies very easily so, you can just write down by using chain rule. So, the first term would become, if you apply a chain rule straightaway. So, this would become the derivative of the partition function times nj plus 1 over Q of the derivative of the occupation number, average occupation number times Q ok.

Of course, by the definition that we have written earlier here, you can substitute for this first term as expectation value ni into what you have as a remainder expectation value of nj ok and realizing that this Q knocks off with this Q ok. But what you have is basically, a derivative of a function; so, average occupation number nj is nothing but 1 over 1 plus e to the power minus beta E j minus mu ok. So, this has to go to 0 because the function does not depend on E i and you are taking derivative with respect to E i. So, this derivative goes to 0 and what you left with is just the fact that these crossed moments. If i and j are not the same is nothing but the product of individual moments. I am sorry so, I must correct myself here. The cross moment is equal to n i n j, that is a first result so, let us sort of save it.

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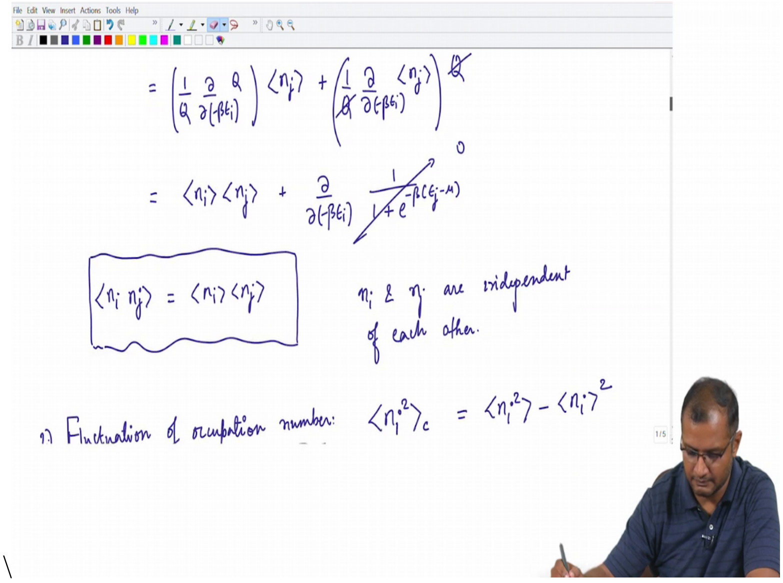

So, this is like the two random variables, which are independent of each other and so, the joint moment is nothing but the product of independent moments. So, in some; at some level you should have seen it coming because these variables are uncorrelated or independent of each other.

So, at some of you may say that I expected this because I know this from chapter 1 on probability where we have computed cross moments of random variables that are mutually independent fine. So, if you realized that this is nothing but a revisit to chapter 1, some of the problems; then, you are on the right track. You have been reading well and doing your homework well.

Another thing that you can compute very easily for the fermions is the fluctuation of the occupation number. So, at t equal to 0, you can see there is no fluctuation all the way to the Fermi surface because the average occupancy is fixed. But at finite temperature you should expect to see some fluctuation of the occupation number near the Fermi surface; where the numbers will deviate from exact 1.

So, let us compute the fluctuation of the occupation number. This is again something which is very simple to calculate. So, if I want to compute; so, this was the first task and if I now want to compute fluctuation of occupation numbers. So, this would be like a second cumulant of some i th; second cumulant of the occupation number of i th level. And we know that the second cumulant can be computed as second moment minus the square of the first moment ok; the simply variance basically, simply variance of the occupation number and n i.

So, we can compute this very easily by simply writing down the right hand side ok. So, the left hand side is basically this and if you recall the definition of; let me just remove this here and so, bring up the definition that has written here. So, we can simply write it here.

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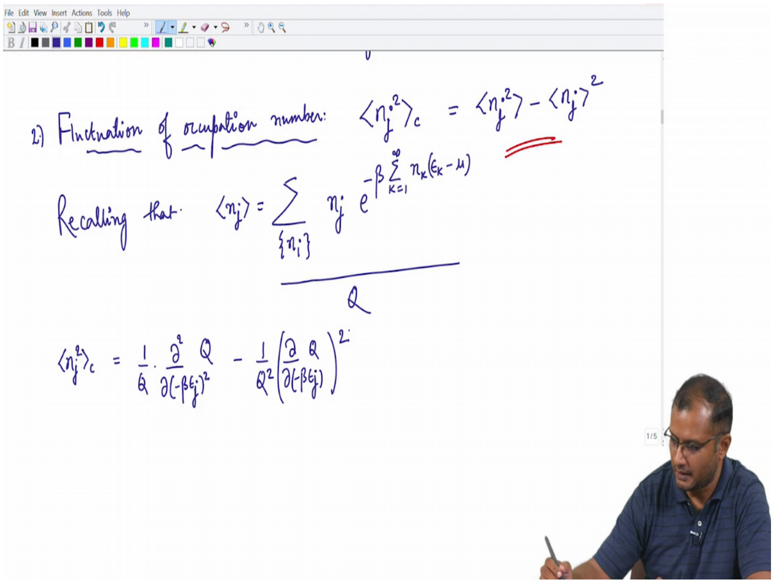

So, recalling that the average occupation n i is nothing but summation over all the microstates ok. And if ni confuses you we can take it as n j; so, how about taking a different symbol? So, we can take a different symbol. So, i average occupation is nothing but the sampling n j in our distribution which is over to partition function ok.

So, then you can see that I can write down the right hand side ok, I can write down this term the; the right hand side here, very simply as. So, let me write down the left hand side first and so, the second moment is now, very easily seen as 1over Q, the second derivative with respect to the j th level of my partition function minus the square of the first moment, which is basically the first derivative.

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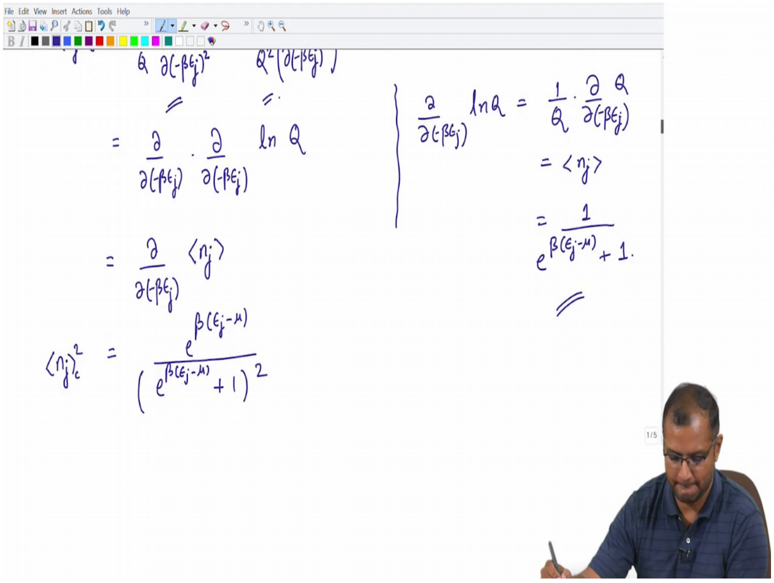

And just to simple rearranging, rearrangement of terms is required here. So, what we can do here is to see for the fact that I can write it as d over; so, we have been doing this many times now. So, you can write this as d over t e i, the second derivative basically of ln Q.

So, as you can see the innermost derivative sort of expands to ok; so, let us sort of explain this, what is going on? So, the inner derivative expands to 1 over Q d over d minus beta i of Q ok. And the outer derivative will give you the first term, which is this; that is the second term, which is this.

Students: (Refer Time: 19:18).

Yeah. So, this is now fine.

Student: (Refer Time: 19:27) should also go replacement (Refer Time: 19:28).

Correct. So, these are typo here; that I have to correct. So, these are both the derivative with respect to E j ok so, I have corrected that typo. So, as you can tell that if you take one more derivative here, you will get your right hand side ok. So, here you can see that this is nothing but by the definition of average occupation number, this is nothing but the innermost derivative is nothing but average n j ok.

Because we know that the average n j is nothing but 1over Q is I think I have already written it here. So, I can simply ignore all that and ok so, this is nothing but average n j ok. And this we know that is nothing but by Fermi Dirac statistics, it is e to the power e raised to beta E j minus mu plus 1.

So, let us then proceed with our final calculation; so, this becomes nothing but if i use this definition so, this derivative can be written as e to the power beta ok the 2 minus sign becomes positive. And so, this is let us not forget for the fact that this is basically, the second cumulant of occupation number.

Student: nj square.

Right.

Student: nj square will (Refer Time: 21:35).

Which one?

Student: left hand side (Refer Time: 21:42).

Yeah, that is what I have written know.

Student: I have written first convention.

Oh ok. So, yeah this is absolutely right, thank you. So, this is the second cumulant ok.

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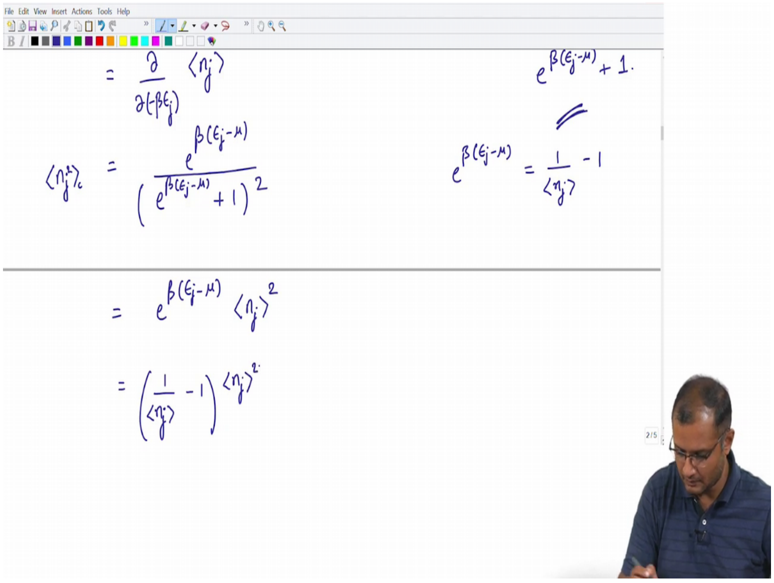

And by substituting the value of the you know, the first of the; for first moment I can easily see that this is nothing but e raised to beta E j minus mu, the denominator is nothing but simply n j square because that is the, that is what is written here. So, square of this is nothing but nj square. But I can also replace this; so, I can also replace for e to the power beta h you know this exponential; I can write this as; so, I can write this as 1 upon nj minus 1 right. So, let me write it here, this becomes ok.

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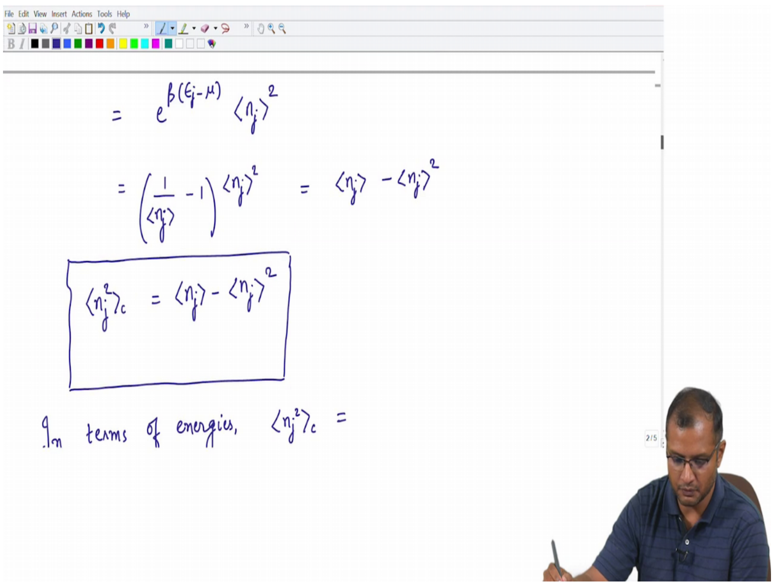

So, in terms of the occupation numbers, you have a neat closed expression which is n j minus n j square ok, right; is that fine. It so, I can also write down in terms of energy. So, this is the expression that we have obtained. So, let me this is an important result; so, let me just put it inside the box. So, this is the cumulant second cumulant of the occupation level; occupation number and it is obtained in terms of the occupation number itself ok. But suppose I want to write down the second cumulant terms of energies ok.

So, if the task is to write down the second cumulant in terms of energies. Then, that is also possible. So, you would like to set up, you consider this plot this is a function of energy. So, you can also write this as in the second cumulant as if I go back and pull down the expression somewhere, yeah it is here. So, I can use this to write it in terms of energy compact form; this can be compactified. So, let us copy it from here and take it downstairs and if I bring it here, I can do something with it; compactify it and yeah.

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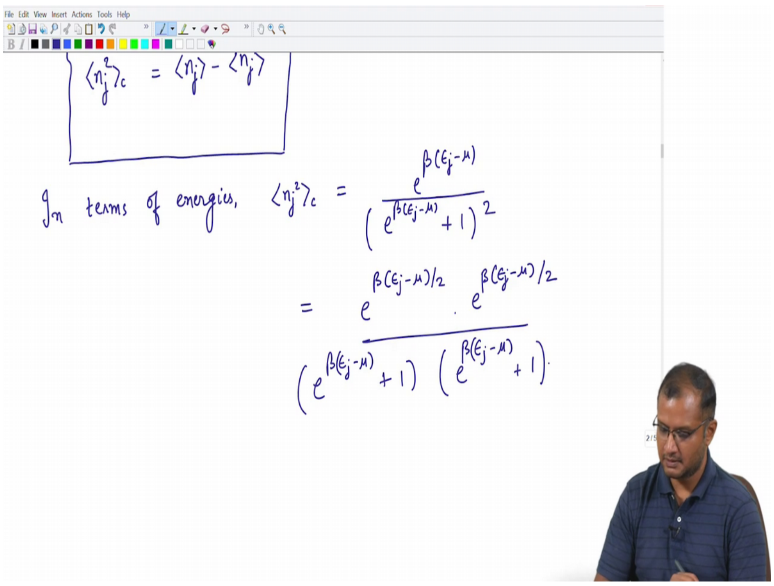

So, I can do something with this; write it in terms of energy. So, realizing for the, you know, I can just rewrite it so, what I will do is; write this as e to the power, the numerator I am going to write down as E j minus mu by 2 into E j minus mu by 2. So, I am writing numerator like that and I am writing the denominator as I just write down the square as you know, as a product of two factors ok.

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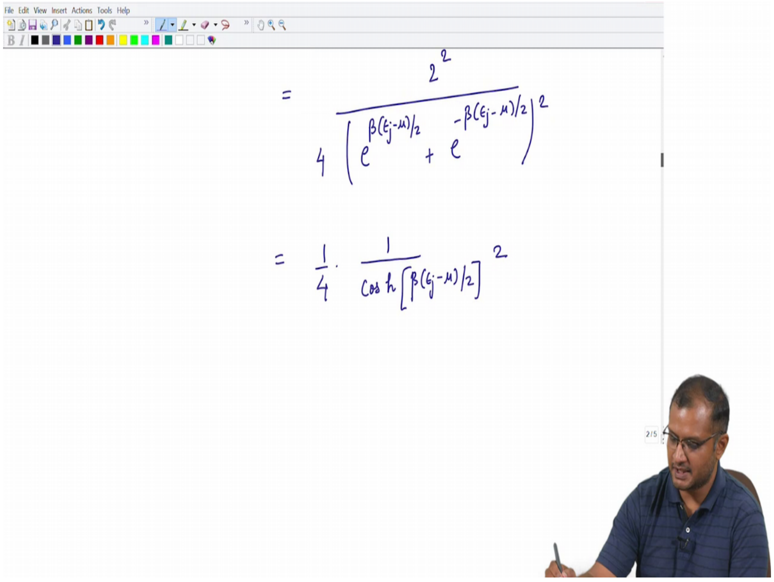

And now, just multiply by the inverse of the numerator. So, I will get a 1 there and each of the numerator factor you divide it in one of the factors in the denominator. So, what you will get is basically e raised to minus; so, what you will get in the denominator is basically, the whole square ok. So, this is; this can be readily converted into cosine hyperbolic. So, what I have to do is basically; now, what I have to do is basically take multiply the numerator by 4 and denominator by 4 and simply, remove this thing from here or let it be like this. We will just write it as 2 and you have write it as 2 square. So, this is like 1 upon 4 into1 upon cosine hyperbolic of beta E j minus mu over 2 the whole square ok.

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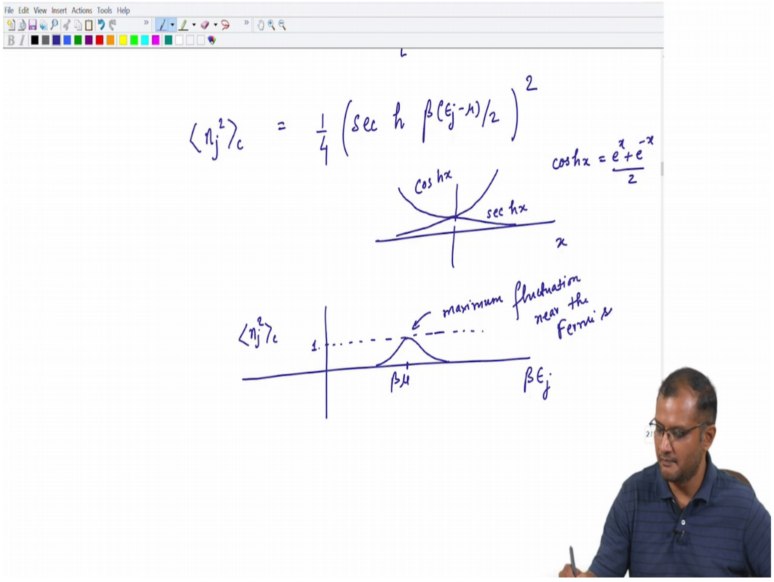

So, this is basically, you can write it as maybe 1 upon 4, a second hyperbolic beta E j minus mu by 2, the whole to the power square so, 1 by cos hyperbolic is second hyperbolic. And you know that so, this was let us not forget the site that, this was of the second cumulant. Now, you have it in terms of energy. So, if you know the plot of cosine hyperbolic; you know how the second hyperbolic would look like.

So, cosine hyperbolic has a plot of something like this. So, if you plot cosine hyperbolic as a function of x then, it will have a minimum at x equals to 0 where, this will be 1 and then, it will go to infinity because cosine hyperbolic has well, you already know by now, but I am just writing it for reference.

So, it logic, it behaves like an exponential and for negative logics also it behaves like a positive exponential so, it goes to positive infinity as x goes to. So, definitely a second hyperbolic has to now, you know it is maximum value has to be 1 and then, it should go to 0. I am not a very good artist so, please bear with me, if you can draw it better than me.

So, I know, I have to just make the infinity go to 0; please draw better than me. This is second hyperbolic because when, cos hyperbolic goes to infinity, it will go to 0. And second hyperbolic square will go even faster than second hyperbolic. So, this would be much faster, it will go to 0. But you already know that it goes to 0 when, x is; so, it is maximum; second hyperbolic is maximum when, x is 0. And our x is actually beta E minus mu; which means, if I want to plot so, if I want to plot beta E j versus the fluctuation.

Then, I expect the fluctuation to be maximum at beta mu and this is where, I will have this passing from 1 and it will quickly go to 0 on both sides. So, when Ej becomes mu, you will have a maximum fluctuation because that is where second hyperbolic 1 becomes 1. So, that is where the fluctuation is maximum and away from it the fluctuation will go to 0, rapidly.

If mu was 0 then, this shift in p could come back to 0, but mu is not 0 and so, you have a maximum fluctuation near the Fermi surface, which is what we expect. Because if you look at your distribution function, this was a t equal to 0, but so, this is at t equal to 0. And if we want to sketch for distribution for non-zero temperature then, this is would we expect the maximum fluctuation to be at close to the Fermi surface, which is somewhere here and that is precisely what you get here. So, I will take this as so, mu at t equals to 0 ok.

So, this is; this completes the discussion on the fluctuations and I think you are now in a position to do most of the problems that are of physical relevance across the three chapters. And if there are any concerns regarding these problems, you feel free to write to us through the Google form that has been uploaded already. And we will be very happy to discuss a issues across the chapters in the live session that is going to come up in the next week.

So, please write to us and talk to my TA in the chat rooms and we will get back to you as soon as possible; in the fastest possible time scale. So, thank you very much, thanks for your patience, we wish you all the best for your exams; upcoming exams. If there is anything we can do, we can fix online just let us know we will try to do our best.