Statistical Mechanics

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Lecture – 16
Statistics of Fermions and Bosons

Good morning students. So, today we will talk about the statistics that distinguishes the two fundamental type of particles that we have discussed in the first class the fermions and the bosons. We saw in the classical statistical mechanics that the particles are all given by Maxwell-Boltzmann statistics independent of whether they are you know independent of the type of the particles. But in the in the quantum world when we are pushing towards high densities and low temperatures, the statistics of these particles are fundamentally different and we will see today why ok.

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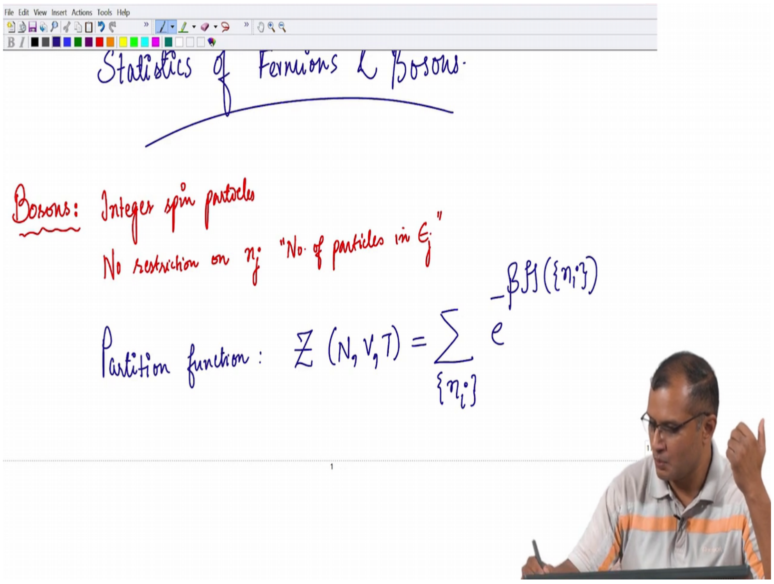

So, the agenda of today's lecture is Statistics of Fermions and Bosons ok. Now, to derive the statistics, I will start with the partition function of system of bosons and fermions that we have discussed in the last class. So, let us take the example of bosons first. So, I am going to take the case of bosons. And, here we have already seen that these are classified as particles whose wave function the wave function of the n particle system or the wave function of the n boson system has an even parity.

So, this essentially means that if I permute the particles in the system the overall wave function does not change its sign. And this has natural consequences on the statistics it follows. And, this is because the evenness of the parity operation allows an arbitrary number of bosons to sit in one energy level, and this is usually represented as the spin being in interior. So, they are classified as integer spin particles ok. And, there is no restriction on the number of particles that can sit in a given energy level. I am going to say that as n j you know the number density or you know it can only be it can be any number between 0 and infinity ok, number of particles in some energy level j ok.

So, I can write down the partition function for this system under constant NVT conditions for n bosons as summation over all the microstates that is the possible you know values of these n i's, which constitute a single microstate. And you sum over all possible values of such a nice into e raise to minus beta the Hamiltonian. So, this is your the Boltzmann factor. What is meant by summation over all possible mm excitations n i? Well, this summation is over all microstates.

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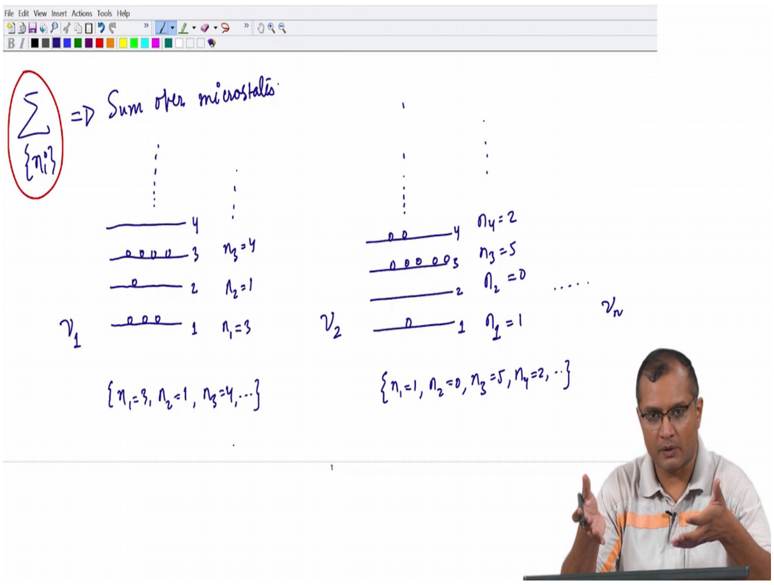

So, let us take off you know take one microstate here. So, the meaning of summation over n i is basically the fact that you know you are sum over microstates ok. So, what is this sum, how is sum implemented, how do we visualize in our heads this sum? Well, you take one microstate. So, I am going to write down one microstate. Let us say I am going to write down microstate mu 1. In this microstate, you could have the energy levels let us say you know you can have energy level 1, 2, 3, 4 and so on.

In infinite energy levels, these are in number of energy levels are not you know they are they are basically uncountably large. And let us say in the microstate mu 1, I am having three boson sitting in the first level, one boson sitting in second, and you know 4 of them sitting here. So, basically for the microstate mu 1, I have n 1 equals to 3, n 2 equals to 1, n 3 equals to 4 and so on, but then the microstate can change I can go to a mu 2 microstate where the population of these levels are different.

So, again the first level, second level, third level, fourth level, and in this case let us say one particle sitting here, nothing sitting in 2, you got 5 sitting here and maybe 2 sitting here. So now, my n 1 is 1, n 2 is 0, n 3 is 5, and n 4 is equal to 2 and so on. So, this way you can change your microstates. So, the summation over microstates that I am I have written here is basically the summation over all possible sets off n i. So, for example, this would be mu 1 microstate would be the set you know with the values n 1 equal to 3, n 2 equal to 1, n 3 equal to 4 and so on.

Then my set of excitations become n 1 equal to 1, n 2 equal to 0, n 3 equals to 5, and 4 equals to 2 and so on. And with the third microstate my set changes, so that is the meaning of summation over all sets of n i. You take one set of a n i's that is constituting your one microstate then the set change. So, you are now looking at a different microstate and so on and so forth.

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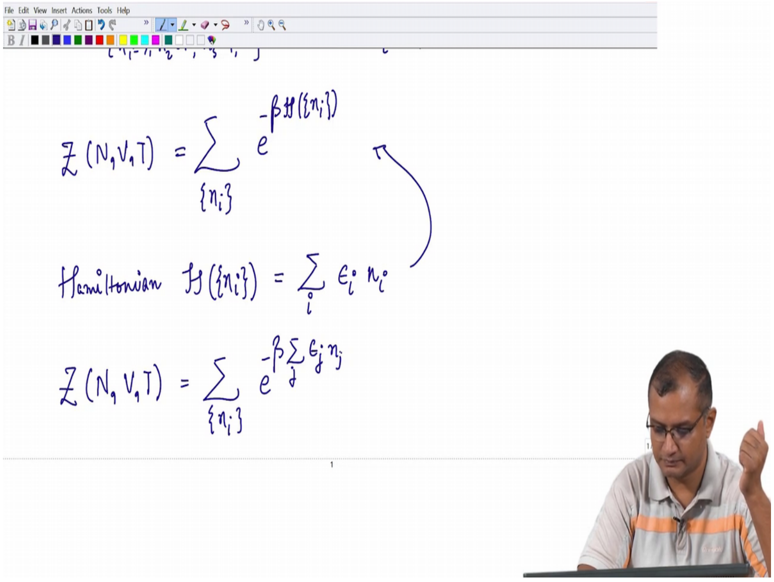

So, that is the meaning of our partition function at constant N V T conditions. So, you have summation over all the set sets of n i's. And our Boltzmann factor was e raised to minus beta the Hamiltonian of that particularly chosen set in the summation ok.

Now, the Hamiltonian of the microstate is given by a nothing but well the energy of the state multiplied by the number of guys sitting in that state ok. I will run from a 1 to infinity, because you have infinite energy levels in the system alright. So, let us plug this value here. And now I can write down my canonical partition function as a summation over all possible sets of n i's into my Boltzmann factor that is I am going to change the label here n j fine ok; j is just the label ok. Suppose, I choose a microstate with n 1 equal to 2, n 2 equal to 3, then for that microstate you compute the Boltzmann factor.

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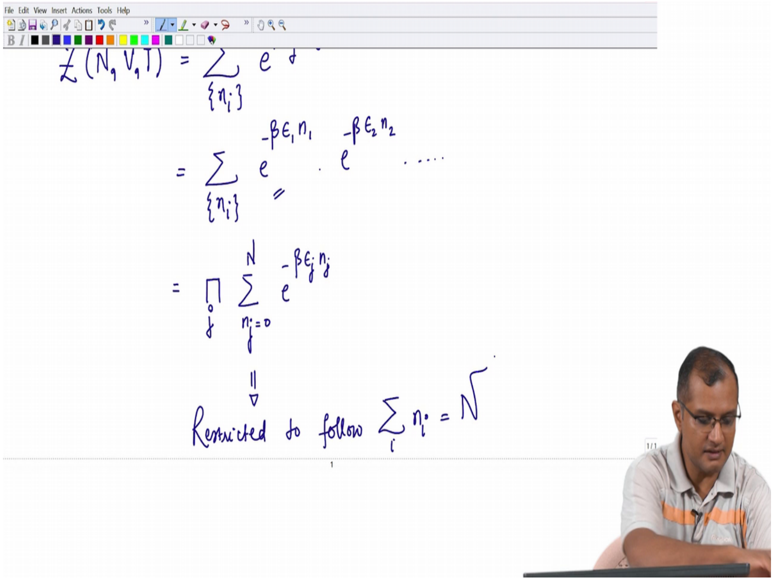

Now, this can be written as e to the power minus beta ok. There are infinite terms here, but there is no a problem, it becomes clear. So, I can write down this as you know the product of these exponents are taken here outside ok, and the sum for each value of j that I take ok, suppose j is 1, then I have this particular thing, but it has to have a sum over all the n i's ok. So, then I will take my n j going from 0 to n because I have n fermions in the system and this is basically e to the power minus beta E j n j and it is very difficult to perform this sum simply because I have a restriction here the sum is basically restricted to follow a constraint the total number of particles.

So, I cannot take n j arbitrarily from 0 to n for sum j, because there is another exponent corresponding to another pi j outside where I can only take the values of n such that the sum of two ns are always constitute or are always constrained to become n. So, this constrained sum is very difficult to perform ok.

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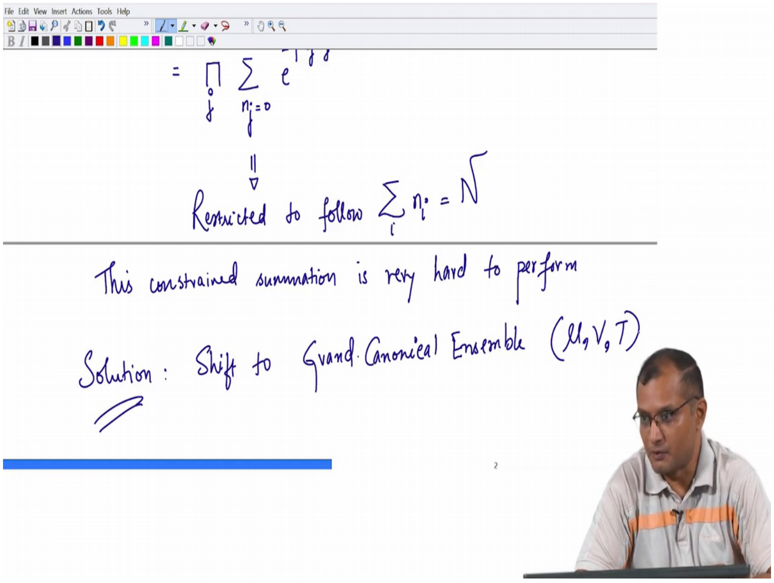

So, this constrained summation is very hard to perform meaning being the label n j which is the occupancy of jth level cannot be independent taken from 0 to n for these exponents. Suppose, I take n j as n by 2 for the first exponential, the next exponential cannot have n j anything other than you know what I am left with is basically I cannot take it as n by 2 plus 1. And I have got infinite number of exponentials there ok. So, for each one of them, the label n j cannot take independent values, they are constrained to sum up to n which is the number of particles in the system. So, I cannot perform this summation it is very hard.

So, what is the solution? So, the solution is to shift the problem to the grand canonical ensemble, where n can change ok, but it will keep the chemical potential constant. So, I am going to go to the grand canonical ensemble, where number of particles in the system can change, this sum becomes unrestricted now, but now I have to conserve the chemical potential.

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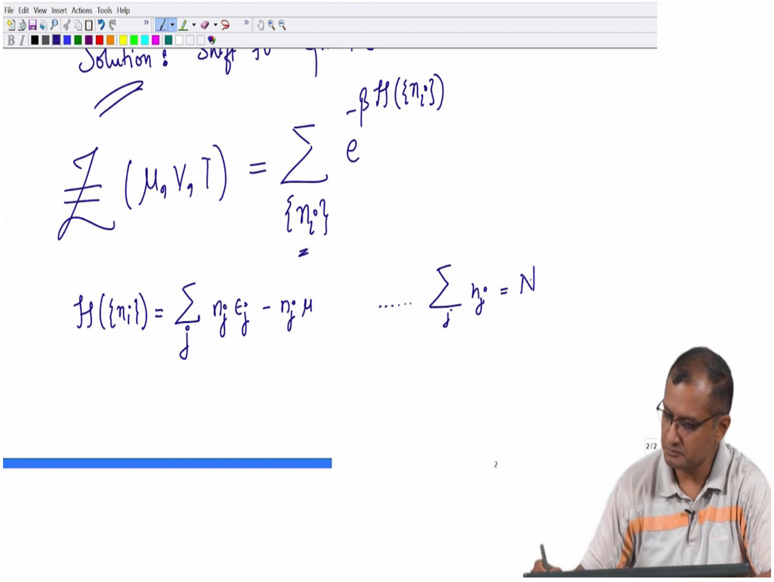

So, let us shift to the grand canonical ensemble which means now I will be computing the grand canonical partition function indicated here by two horizontal crosses on the function Z. And as usual here I am going to write down my partition function as summation over all the microstates into e raised to minus beta a Hamiltonian of the microstate that is chosen by the summation here ok.

Now, the Hamiltonian of the microstate in the grand canonical ensemble is nothing but summation over all the values of energy levels times the excitation of this level or number of particles sitting in that level and multiplied by energy of that level minus n j times chemical potential, because we have taken summation n j as n, n for that particular microstate because n itself is now changing ok.

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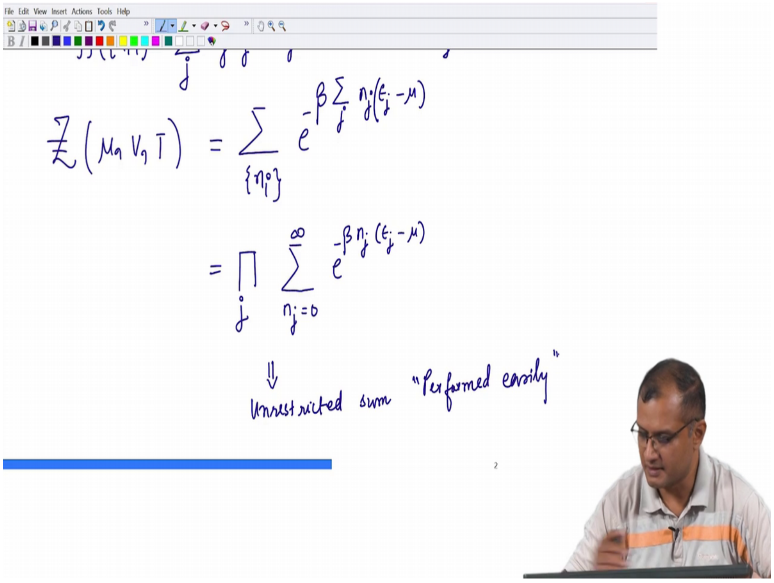

So, if you plug this in the above expression our grand canonical partition function now becomes summation over all the microstates e raised to minus beta and I am plugging the Hamiltonian here summation j n j into E j minus mu ok. As usual the exponent is a sum ok, so that becomes product outside ok. So, then I have for each j, I will now take an unrestricted some. So, this is the meaning of the unrestricted sum here.

Now, for each exponential my n j can go from 0 to infinity ok. And this will be e to the power minus beta ok. So, now, you have no problem. So, this is now an unrestricted sum. So, I can take in each exponent my label going from 0 to infinity which I could not do previously. So, if you take is 0 to infinity, then you can you cannot do anything in the second one, because you are n has been you know you have to conserve the total number of particles.

But here I do not have to conserve my number of particles my n could be actually infinity to go up to infinity which means each n j which is independent of the other exponent can run from 0 to infinity without getting affected by the label in the next exponent. So, this is how I understood sum which can be performed very easily, because I am not conserving number of particles anymore ok. Then the grand canonical ensemble number of particles is not conserved. What is conserved basically chemical potential volume and temperature and that allows us to compute the sum in an unconstrained manner which we could not do previously.

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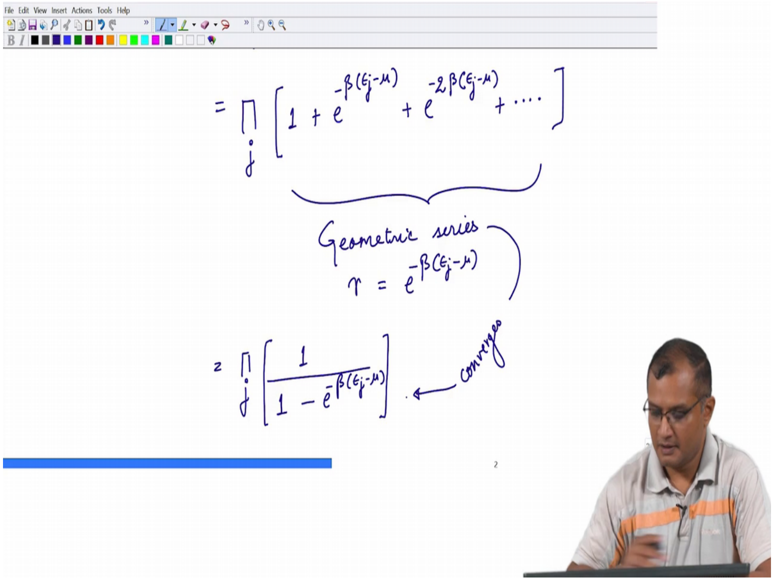

So, then I can write down this as a just pi j sum over all the j's and for each j that I set outside I am going to write this sum inside for a few terms. So, I am going to take the first term for j equal to 0 and j equal to 0 is 1 then the second term is minus beta E j minus mu when n j becomes 1; and for the third term, it is e raised to minus twice beta and so on. You have infinite terms here ok. As you can see this is a geometric series with the common ratio r as e to the power minus beta E j minus mu.

And the ratio of the successive terms in the limit n going to infinity converges for any value of beta E j n mu. So, this sum converges to the closed form 1 upon 1 minus the common ratio which is e raised to minus beta E j minus mu that is the converged sum fine.

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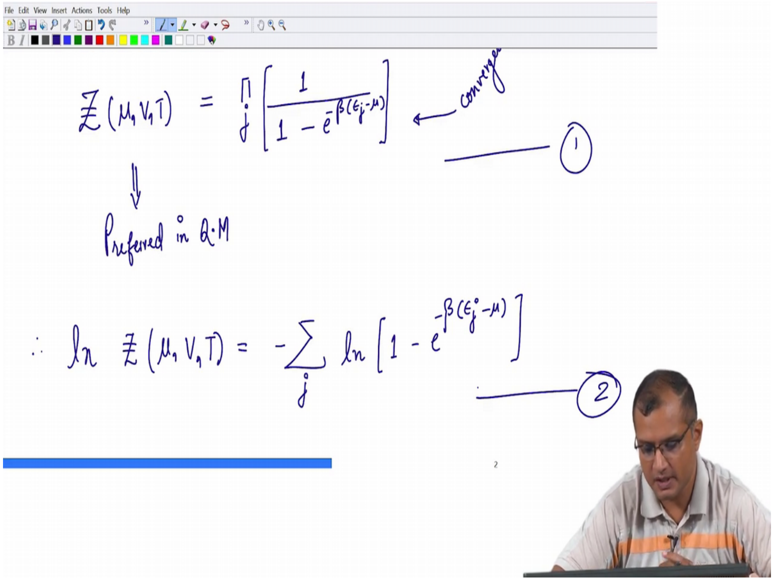

So, now, I can realize this as my grand canonical partition function, and grand the for the fact that you know the number of particles was not conserved and I could perform this sum in the partition function in the unconstrained manner. So, before we proceed further we would like to state here that the grand canonical ensemble is hence the natural choice of ensemble when you are doing quantum statistical calculations. So, when people say it is the ensemble to do correct enumeration of states, well they are also saying this because it is also more convenient to compute the partition function.

So, the fact that I could enumerate the stage properly which is due to the fact that the sum was performed in an unconstrained manner makes the grand canonical ensemble a preferred choice for doing the calculations ok, so that is why this is the preferred ensemble when you are doing quantum statistical mechanics. So, then let us take a logarithm on both sides, which will be using it in the correspondence between classical to between quantum and classical statistical mechanics.

So, let us just make a small note of the result. If you take logarithm on both sides, what we get is nothing but minus the logarithm of a the products become sum. And, so let us say that this is the result 1 and that is the result 2. So, we are now in a position to compute or to form these statistics of bosons. So, this discussion was for bosons. So, I am going to derive the average occupation number of bosons in some energy level j ok.

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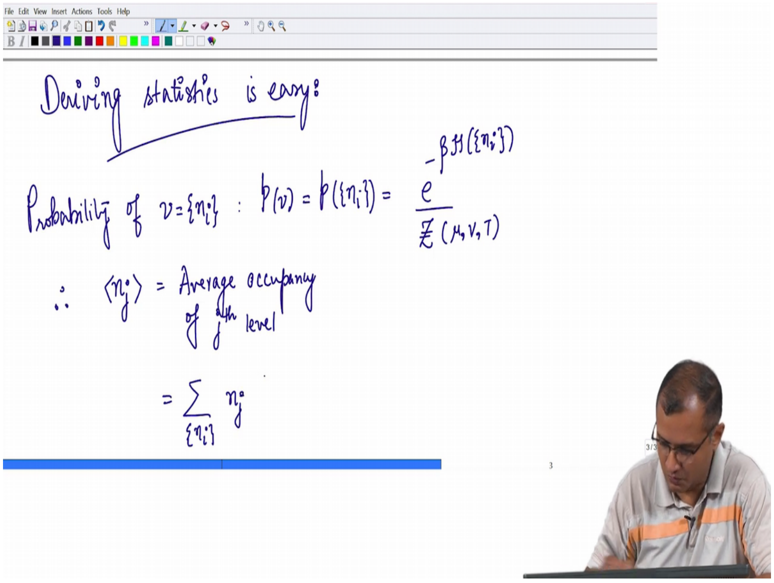

So, deriving the statistics is now very straightforward. It is very easy now. And since you have followed the lectures in the first two chapters, you know how to compute average of any quantity if you know the distribution function in that corresponding ensemble. So, I know that my partition function is represented here either you can take expression one or you can take the first expression here ok.

So, I am going to write down the, if I know the partition function then certainly I know the probability of finding the microstate n i ok. So, certainly I know the probability of a microstate some collection of these n i's is basically p of mu or p of these n i's which constitutes a single microstate. And the probability of this single microstate is nothing but e raised to minus beta the Hamiltonian of that microstate ok.

So, therefore, if I want to know the average occupancy of sum jth level ok, this has to be normalized to the partition function otherwise you do not sum these probabilities to 1 of the jth level. So, suppose I am interested in the average occupancy in the jth level then this is nothing but summation over all the microstates.

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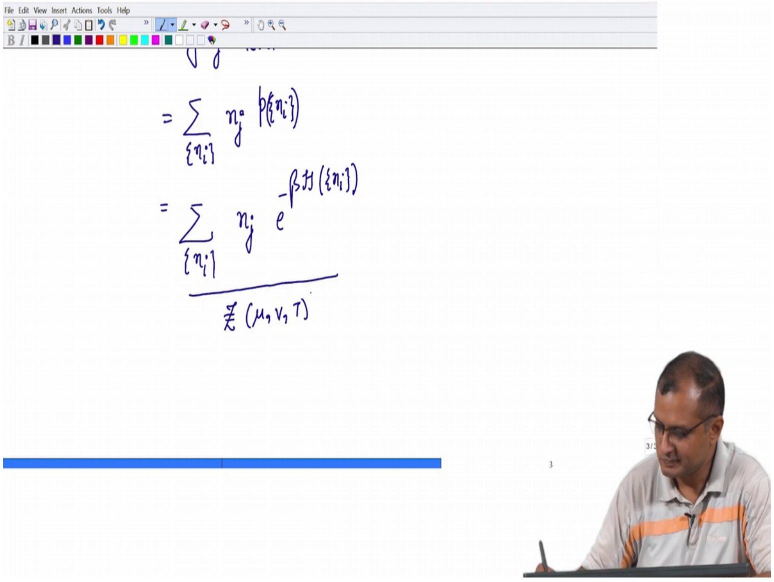

And what you essentially want to find out into so this means you want to basically compute this sum over all the microstates, but you are interested in only the jth level number dense in the jth level into e raised to minus beta. I am now going to plug the form of the probability here which is this ok. So, plug its form, it is e raise to minus beta for sum microstate that is summed over here divided by the grand canonical partition function.

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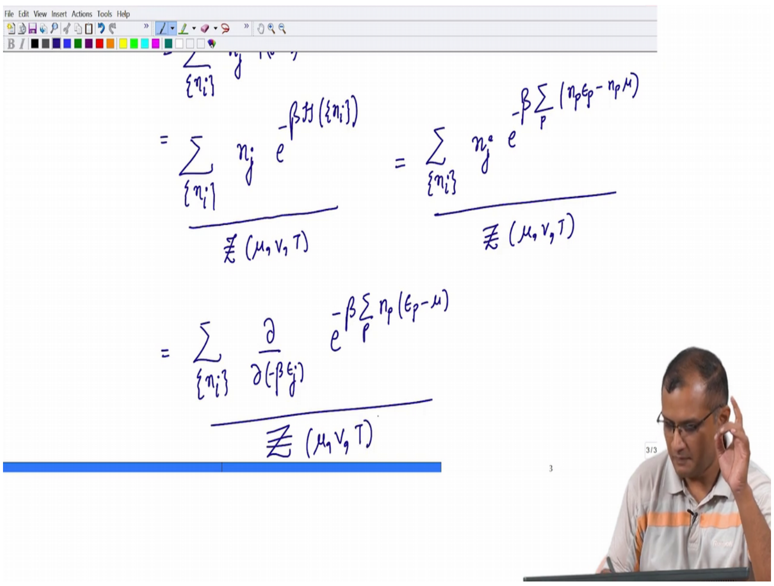

And this is very clear now. If I want to pull out a certain n j from all possible values of n j then all I have to do in fact it will become clear if I write down the Hamiltonian explicitly. So, the numerator is nothing but summation over all microstates n j e raise to minus beta summation over some take a label p and you ray take your n p e p minus n p into mu divided by ok. So, the n p's in the exponents are basically the value set by the microstate that you are choosing you will sum over all the microstates. Now, if I want to pick the jth microstate nj then I have to take the derivative with respect to because in the summation in the summation here.

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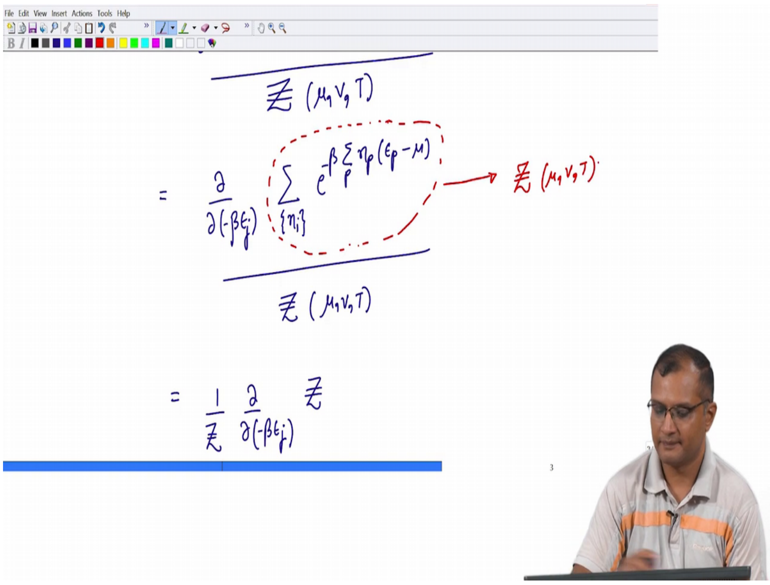

There will be one value of this p, where p becomes j only that value of n j will be taken out when you are taking derivative with respect to beta times E j all other values will go to 0 when they are taken derivative. So, I can write this as d over I can say that this summation is running over all microstates. So, I can simply take the derivative outside because it is for a fixed value of the state and this is nothing but fine.

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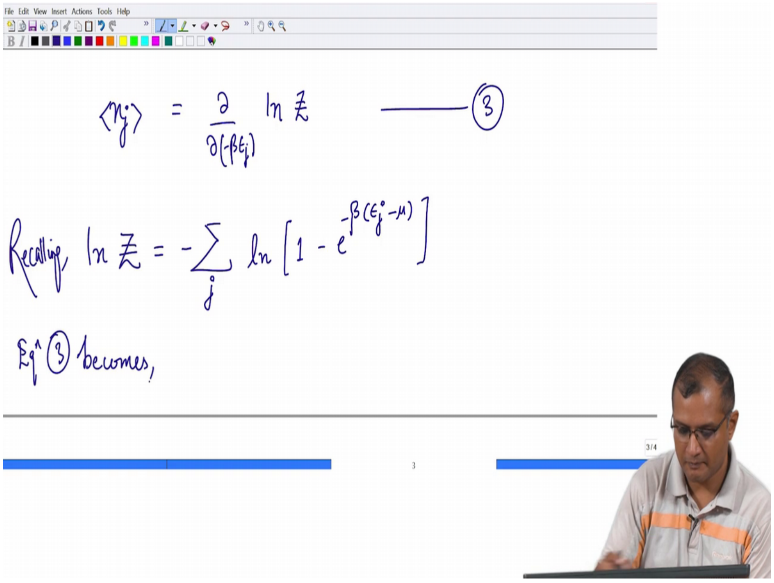

Now this is nothing but 1 upon Z d over minus d beta E j of Z. So, I can call this as the derivative of ln Z ok, because this quantity here is nothing but the partition function itself sum over all the microstates e raised to minus beta into Hamiltonian ok. This quantity is the canonical grand canonical partition function ok, so that is what I have done here.

And now I can say that this is the expression for my average occupancy of the jth level. Let us call this is equation 3. And just plug the value of ln z from here ok. So, because this is a lengthy expression I am just going to copy it here, so that you remember it ok. So, this is the expression for ln z. So, recalling that ln Z is given as negative summation over ln 1 minus e raised to minus beta times E j minus mu. I can take the derivative and obtain n j, average value of n j ok.

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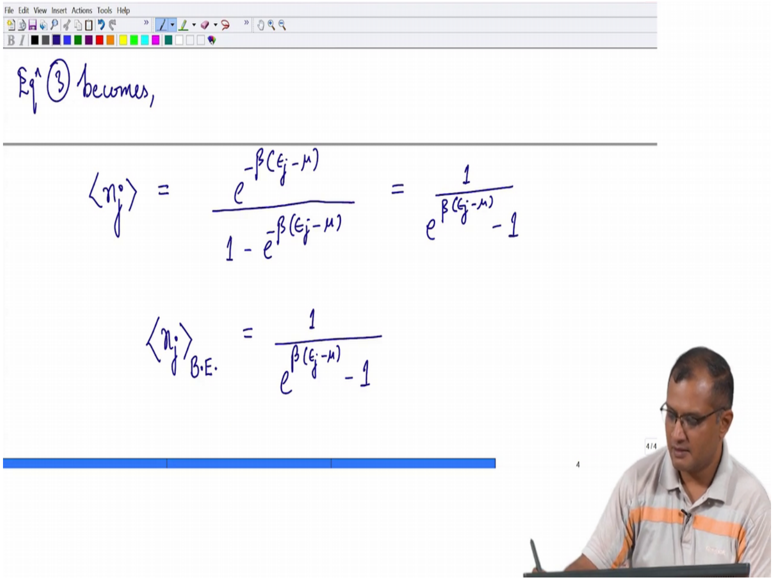

So, let us do the finish this derivative. So, I can write down for n j as only one term in this summation will contribute ok. So, we will have a minus sign outside over 1 minus e raise to minus beta ok. And this minus will turn to plus, and what you will have is just e to the power minus beta E j minus mu. And you can simply write this as 1 over e to the power minus beta E j minus mu.

We can no need to write the plus sign here minus 1. So, this is the Fermi-Dirac this is the bosons statistics which is called as Bose-Einstein statistics. So, I am just going to write down B E to remind the user that this is the Bose-Einstein statistics for the system of bosons ok.

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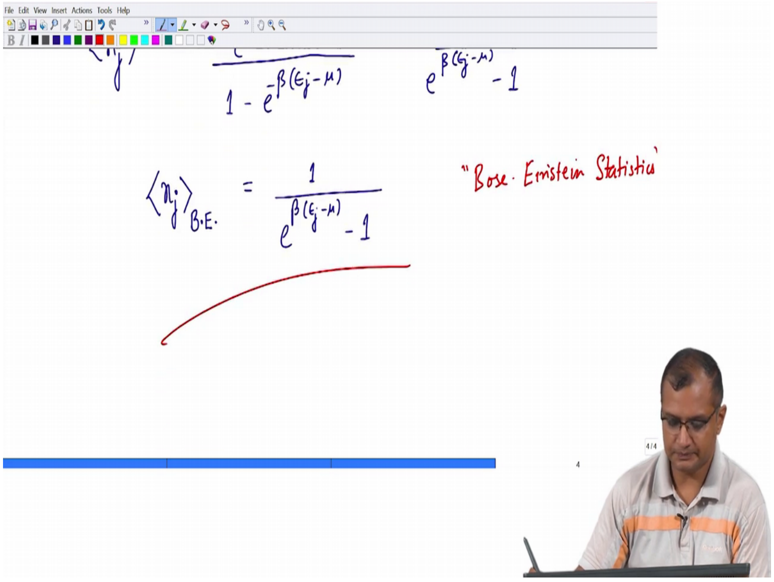

So, this is going to be a very important result that well be using in subsequent lectures. A deriving the statistics for fermions is also straightforward ok.

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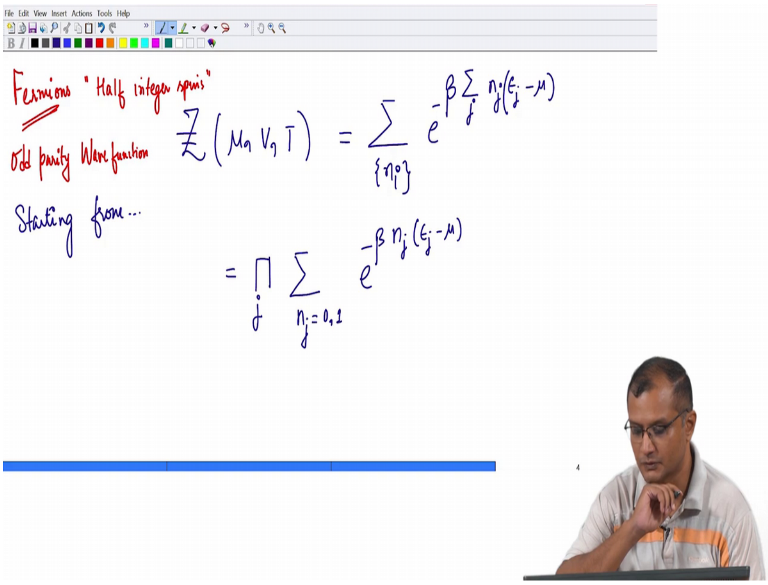

So, you can derive for the system of fermions in a very straightforward manner. For fermions, we will have to start with the fact that the partition function in the grand canonical ensemble of course is still written by and this expression. So, I am going to write down our partition function without altering much. So, so here you can start from the same partition function.

So, starting from the expression for the partition function in the grand canonical on symbol you have to do this derivation slightly carefully in the sense that now you are not expecting the system to you know to show more than one particle in a given energy level. So, the occupancy can be only 0 or 1 for a given energy level ok. So, basically these are particles with integer spins a half integer spins ok. So, the spins here are I will say these are in the vein of previous discussion the spins are half integer

And I am going to say that these are particles whose system has a wave function that is anti-symmetric in nature. So, the fermionic wave function has an odd parity. So, I am going to write this as a reminder here. And then I will say that we are starting from the same partition function except for the fact that when you write down the summation on the right hand side as a product over all the j's, the summation on each n j is now taking values only 0 and 1 instead of going from 0 to infinity this will now take on the values 0 and 1. So, e to the power of minus beta into n j E j minus mu will take the values only n j as 0 and 1 ok.

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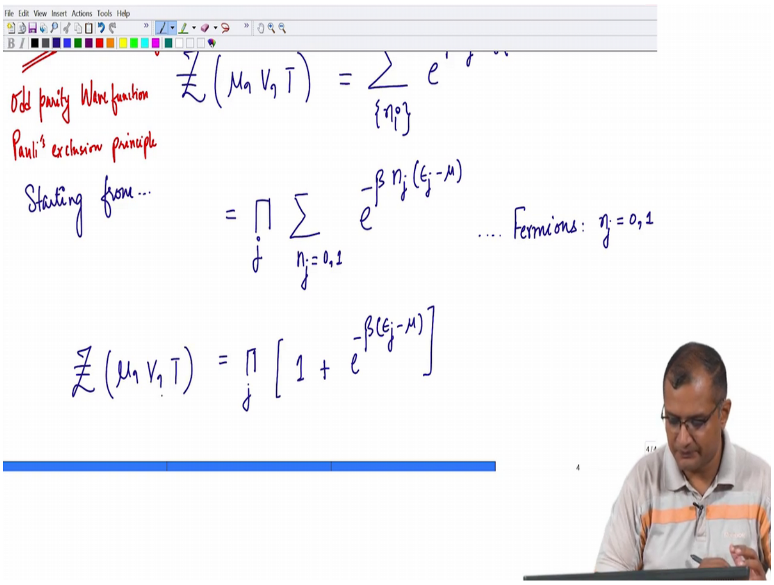

So, then if you write down then what you get here is nothing but pi j. So, keep in mind here that for fermions because of the Pauli's exclusion principle ok. So, you may want to like we wrote in the previous discussion that the oddness of the parity operation on this system results into Pauli's exclusion principle ok.

So, this is the systematic discussion that we have already done in the first lecture that the two systems bosons and fermions differ from each other in the in the sense that one system has a wave function that is that has an even parity the system of bosons. And the system of fermions has an odd parity which means the parity operator for fermionic wave function has an eigenvalue minus 1, whereas the parity operator for the bosonic wave function you know has a bosonic systems has an eigenvalue plus 1. This basically means the following that every time you permute two particles in the fermionic system then the overall wave function incurs a negative sign.

So, that basically means that you cannot like we saw in the last lecture you cannot take two particles to be in the same level because that would make you slater determinant to be 0 and that is the manifestation of Pauli's exclusion principle that you cannot your wave function will go to 0 which means you cannot see a realization where two particles are sitting in the same level. It will make your wave function to go to 0.

So, the system of fermions half integer spins because their odd parity wave function and they follow Pauli's exclusion principle leads us to this definition of the grand canonical ensemble. So, we are doing the statistical mechanics purely from the directions from quantum mechanics and that has led to this stage.

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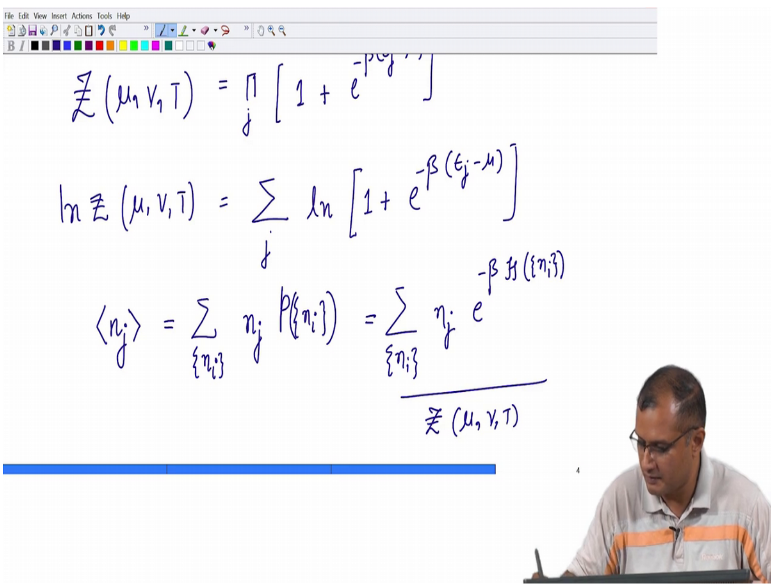

And I can now take the logarithm of this. And this would be nothing but summation over j's ln plus e raised to minus beta E j minus mu. So, therefore, as usual if somebody is interested in the average occupancy of fermions in some level j, then this is nothing but summation over all microstates, I need to sample n j in this distribution of microstates ok. And as before I know that this is nothing but e to the power of minus beta the probability of finding a system in a microstate is given as the Boltzmann factor divided by a partition function. So, this is my Hamiltonian divided my by a by a partition function ok.

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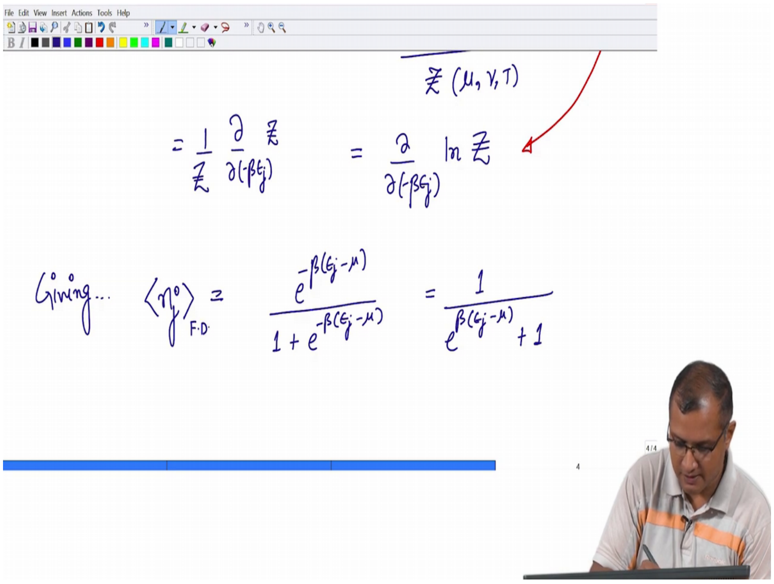

And hence mathematically this is nothing but 1 upon partition function d over minus beta E j as before the partition function. So, this is nothing but d over d minus beta E j of logarithm of the partition function. But now I will use the derivation of the partition function in the system of fermions. So, I am going to use this expression for ln Z ok. So, plugging this expression in ln Z, what do I get ok. So, I am going to plug this for this ln Z B. So, it will give me what is my left hand side and please look at ln Z here.

So, in this summation only the jth term will contribute j is running from 0 to infinity the infinite energy levels in our system of that out of those infinite levels only one level j will contribute to this derivative and that will give me 1 plus e raised to minus beta in the denominator. And I will have a e raised to minus beta E j minus mu in the numerator and just multiplying and dividing by a common factor. I can write this as e raised to beta E j minus mu plus 1; so, then just to remind our self this is nothing but a Fermi-Dirac statistics.

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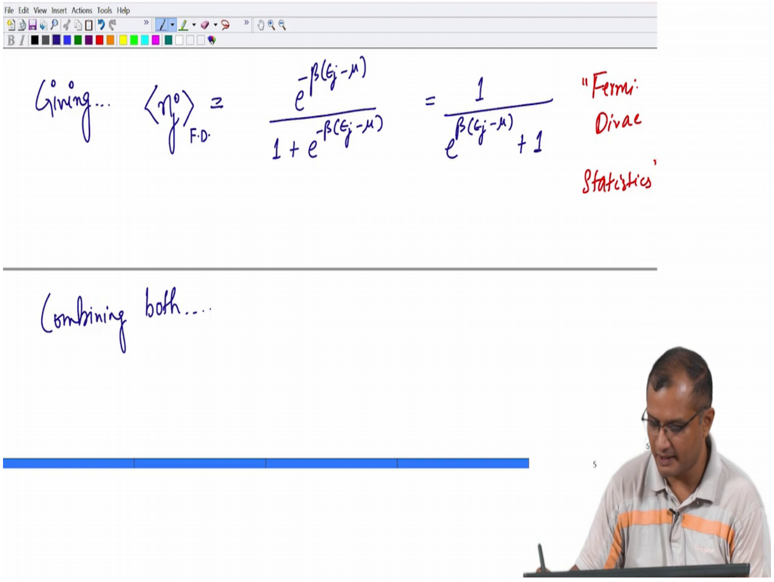

So, I can write this as combining both the results of the Fermi-Dirac and the Bose-Einstein statistics, I can write down combining both of them. So, let me call this as some equation so far yeah combining. So, I am going to call this as Fermi-Dirac.

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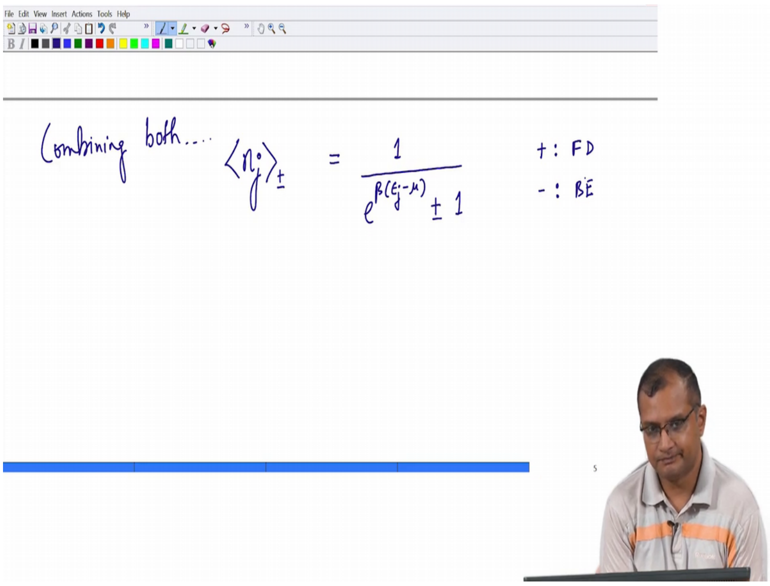

So, combining both of them I can finally write down a single expression for the average occupancy of the jth energy level as Fermi-Dirac or Bose-Einstein as I can in fact, it is better that I use a plus minus ok, so plus for bosons and minus for fermions. I can write it as 1 upon e raise to beta E j minus mu plus minus 1 ok.

So, plus here corresponds to Fermi-Dirac statistics and the minus corresponds to Bose-Einstein statistics ok. So, fine, so this comes so this brings to the end of our discussion on the Fermi-Dirac statistics. And when we meet next time and we will talk about how these statistics decide the heat capacity of a solid at low temperatures due to both the vibrations of lattice ions and the free electrons of a conductor such as you know a copper, where we will see that the lattice contribution due to ions is proportional to T Q and the free electron contribution is proportional to T.

And this is a consequence of the Fermi-Dirac statistics and the Bose-Einstein statistics that these electrons which are fermions follow and the phonons which are the quantum of vibration of vibration of these ions follow. So, these two constituents ions and electrons satisfy different type of statistics. And, hence their contribution to the overall heat capacity of our low temperature solids are very different. And we shall see this in the next lecture alright.