Statistical Mechanics
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Lecture - 32

Canonical Ensemble Einstein Solid

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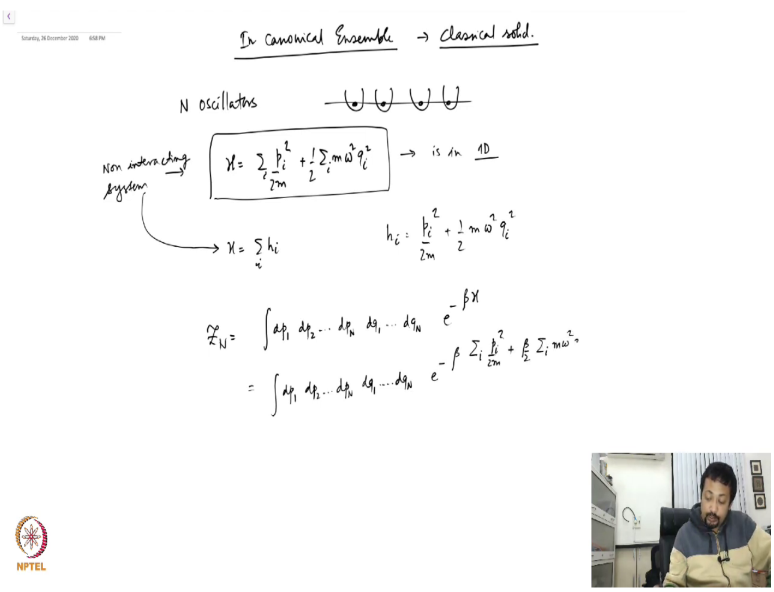

So, now we take up the final example in the Canonical Ensemble and this corresponds to what is called a classical Solid. We have looked at it in the micro canonical ensemble and I have N oscillators, which are essentially lying on a one dimensional lattice and they have been confined by a harmonic trap. So, that the Hamiltonian is given by p i square over twice m plus sum over i half m omega square q i square.

Now, this as we have said before is in 1D one dimensional space the generalization to higher dimension is not a very complicated problem. So, the Hamiltonian i can write down as sum over i h i, so this is a non interacting system and consequently I can write down the Hamiltonian as sum of single particle Hamiltonians; where h i is p i square over twice m plus half m omega square q i square.

The N particle partition function is dp 1, dp 2, dp N, dq 1 to dq l e to the power minus beta h bar which becomes dp 1, dp 2 all the way to dp N and you have dq 1 to dq N e to the power minus beta sum over i p i square over twice m plus beta by 2 sum over i m omega square q i square.

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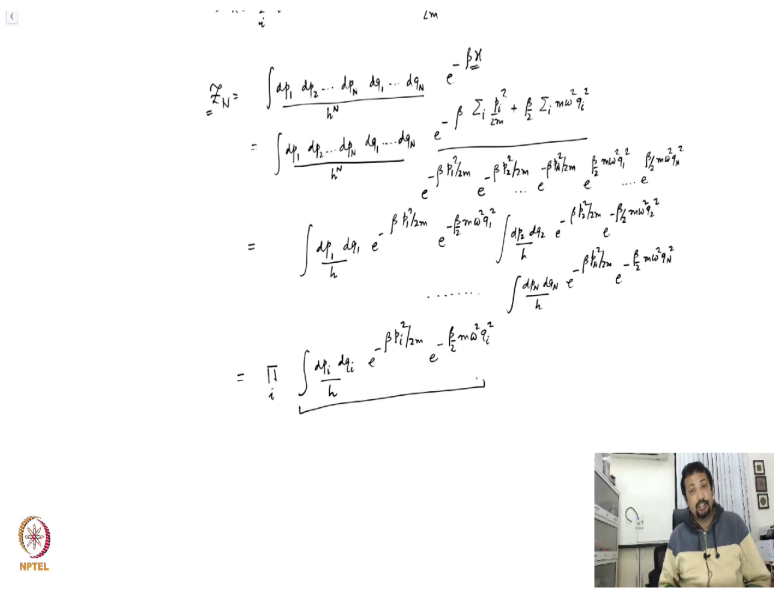

Now, clearly this sum if I write down explicitly becomes product of exponentials. So, that I have minus beta p 1 square over twice m e to the power minus beta p 2 square over twice m and then I have minus beta p N square over twice m I have eta beta by 2 m omega square q 1 square and then finally, I have beta by 2 m omega square q N square.

So, hence I have dp 1 e to the power minus beta p 1 square over twice m. But before we proceed one has to be careful because this quantity is dimensionless, this quantity is dimensionless because the Helmholtz free energy is going to use log of this partition function but this measure is not right. So, that I have h to the power N that must come and sit over here.

So, let us now group the terms together I have dp 1 dq 1 over h, e to the power minus beta p 1 square over 2 m e to the power minus beta by 2 m omega square q 1 square. Then I have dp 2 dq 2 over h e to the power minus beta p 2 square over 2 m e to the power minus beta by 2 m omega square q 2 square so on and so forth.

All the way finally, when I have dp N q N over h e to the power minus beta p N square over twice m e to the power minus beta by 2 m omega square q N square. I want to compactify my notation, so that essentially I will write this as product over i dp i dq i over h e to the power minus beta p i square over twice m and then I have minus beta by 2 m omega square q i square.

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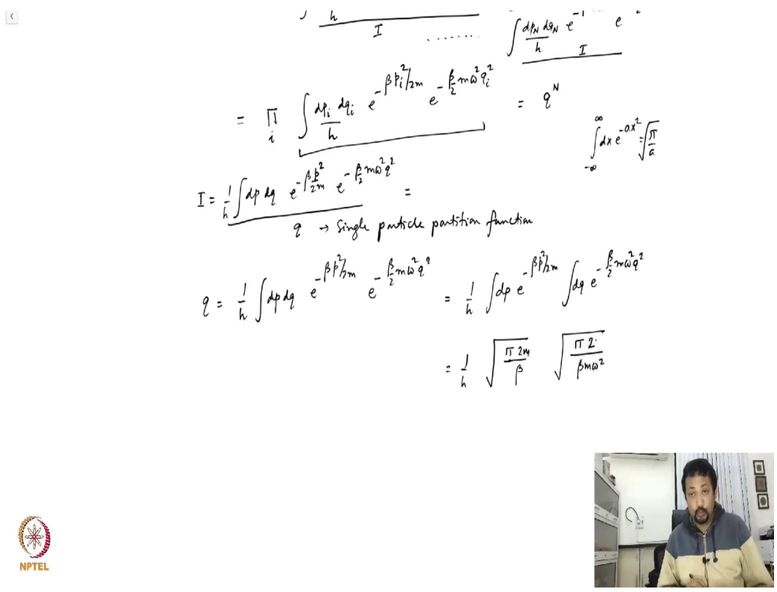

Now, this integral that you see is a Gaussian integral and effectively in the earlier equation you can see that this is a product of N Gaussian integrals where I write down i as dp 1 over h dp dq e to the power minus beta p square over twice m e to the power minus beta by 2 m omega square q square.

And all of this integral is going to give me i i and all the way over high and if you see that this is nothing but the single particle partition function q. So, this is the single particle partition function and the N particles would partition function would be q to the power N. Here again I do not have a N factorial why because essentially I mean I can distinguish the particles by their mean position.

So, let us evaluate this integral let us evaluate q is 1 over h dp dq e to the power minus beta p square over twice m e to the power minus beta by 2 m omega square q square which is going to be, I can separate out the integrals minus beta p square over twice m dq minus beta by 2 m omega square q square.

I use the integral the Gaussian integral minus ax square is going to be pi by a square root of that. So, that the first term is going to be square root of pi over twice m by beta and the second integral is going to be pi divided by beta m omega square times 2.

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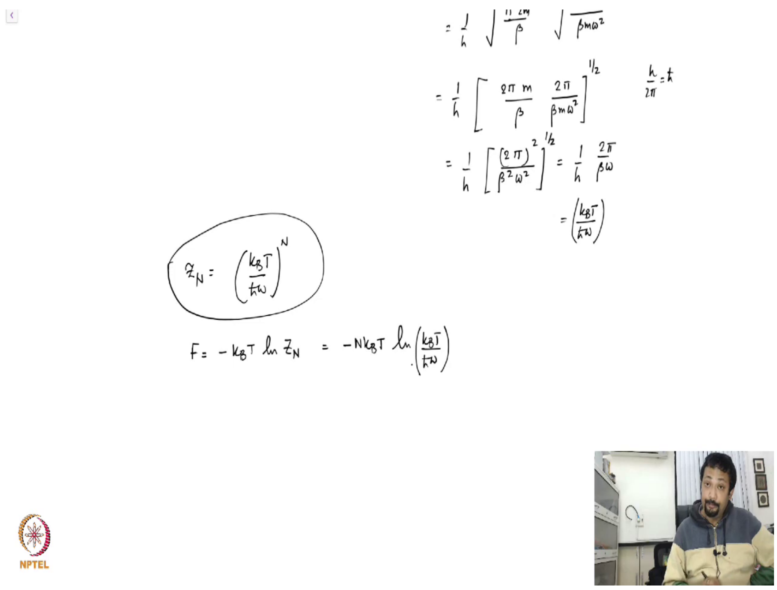

So, if I bring everything together then I have 2 pi times m beta and I have 2 pi times beta m omega square. And then essentially I have raised to the power half, which gives me 1 over h 2 pi whole square beta square omega square and that is essentially raised to the power half and that you are going to get as 1 over h 2 pi over beta omega.

But this answer is very familiar because h bar h over 2 pi is h bar, so that I have k B T over h bar omega. Hence the N particle partition function Z N becomes k B T over h bar omega raised to the power N it is dimensionless because you see k B T has the dimension of energy and so does h bar omega. The Helmholtz free energy is minus k B T l m of Z N which is if I use this expression for Z N becomes minus N k B T ln k B T over h bar omega.

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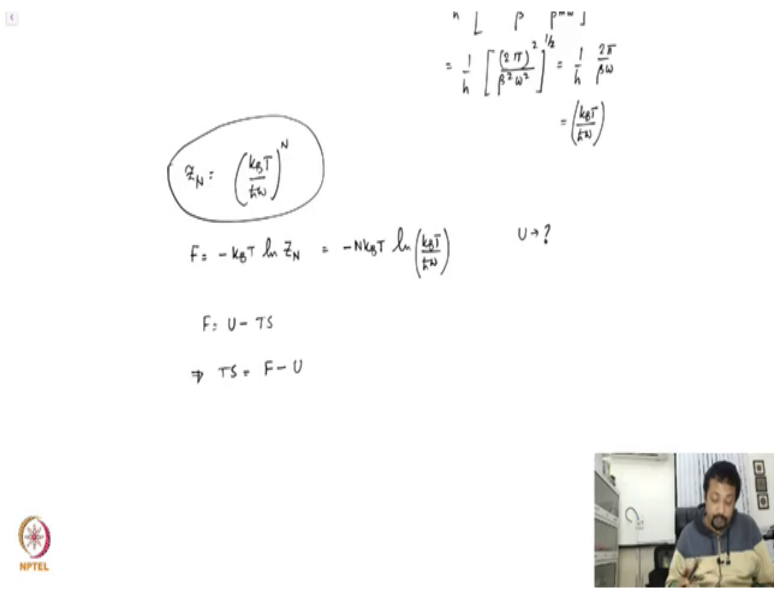

Now, one can determine the entropy from this relation how do you determine the entropy? When we know the root F is U minus TS. And I have to figure out what U is going to be and therefore, this would imply that TS is going to be F minus U, am I right?

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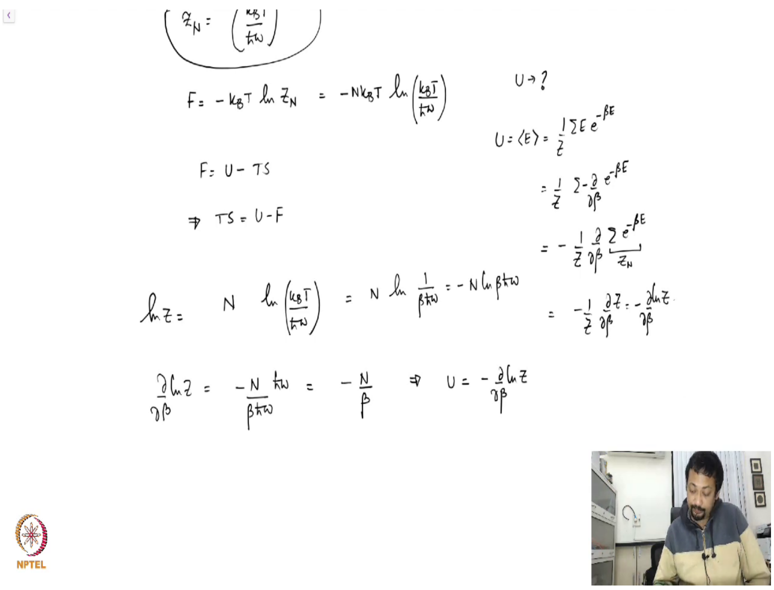

U minus F is going to be; U minus F is going to be TS right. As we have seen the average energy which we identified with U, so U is equal to the average energy of the system which was sum over E in the canonical ensemble minus beta E 1 over Z. And this means that I can do rewrite this expression as del del beta of e to the power minus beta E with a minus sign which means I have minus 1 over Z del del beta of sum over e to the power minus beta E.

And this quantity is the partition function that we are looking for, so I have minus 1 over Z del del beta of Z which is minus del del beta of ln of Z. ln of Z in our case is N k B T ln k B T over h bar omega. No there is no k B T factor I am sorry, it is just going to be N times ln of this; which I will write down since I have a derivative with respect to beta I am going to write down as ln 1 over beta h bar omega, which is minus N ln beta h bar omega.

Now, this gives me a del del beta of this ln Z gives me minus N over beta h bar omega times h bar omega which is minus of N over beta. And this implies that U is going to be minus del del beta of ln Z which is going to be N k B T, the result which we obtained in the micro canonical and symbol also.

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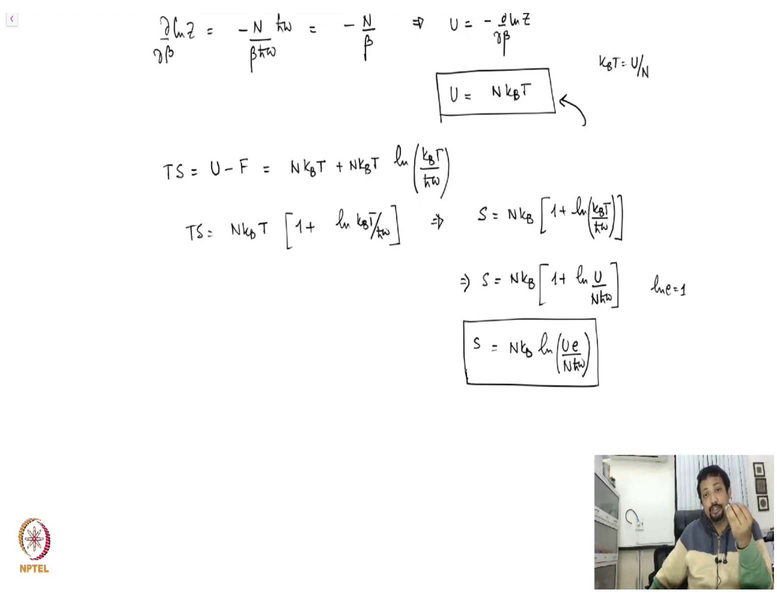

Now, TS then becomes U minus F. So, that I have this is as N k B T and F was minus N k B T, so that this becomes N k B T ln of k B T over h bar omega. Clearly I can take N k B T outside, so that T S becomes N k B T 1 plus ln k B T over h bar omega. And this you see is going to be this implies that the entropy is N k B 1 plus ln of k B T divided by h bar omega.

Now, I look at this expression that I have over here k B T is U over N. So, that this expression implies that S is going to be N k B 1 plus log of U over N h bar omega; which means; I can write down this as N k B ln of U times e where ln e is going to be 1 divided by N h bar omega.

And this is the expression that we have derived in the micro canonical ensemble from the total number of microstates. So, everything fits like a jigsaw puzzle. With this we come to the end of canonical ensemble and next we are going to look at a different canonical ensemble which is essentially where you allow fluctuations in particle number as well as energy.