Statistical Mechanics
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Lecture - 25
Example of Microcanonical Ensemble- Magnetic System and Ideal Gas - Part II

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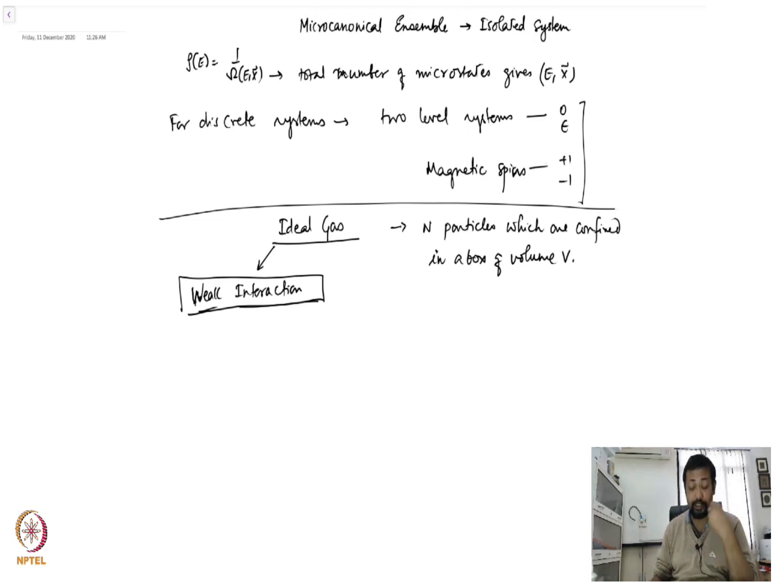

So, we were looking at the micro canonical ensemble which as you recall we said it is for an isolated system. And the density of rho E was 1 over omega E comma x. This is the total number of micro states the omega of microstates given E comma x the generalized coordinates and the energy.

Now, the examples that we did in the last two lectures was for discrete systems. So, we looked at two level systems which were of main interest and correspondingly I mean the in one case we had 0 and epsilon; and we had then in the second case we had the magnetic spins, spins which could take plus 1 and minus 1 values.

Now, we want to look at the case where my microstate can take continuous values, the ideal gas. Here the of course, you are familiar with the picture that we have N particles which are confined in a box of length or let us say a box of volume V. So, an ideal gas is the one where you do not have any interactions actually this is not a right statement, but essentially you have weak interaction, so that you can neglect them right.

So, one should not say that an ideal gas is without in the without any interaction inter, particle interaction, but your state point is such your thermodynamic state point is such that the interaction is very very weak for example, your density can be very less, the temperature can be very high, so on and so forth.

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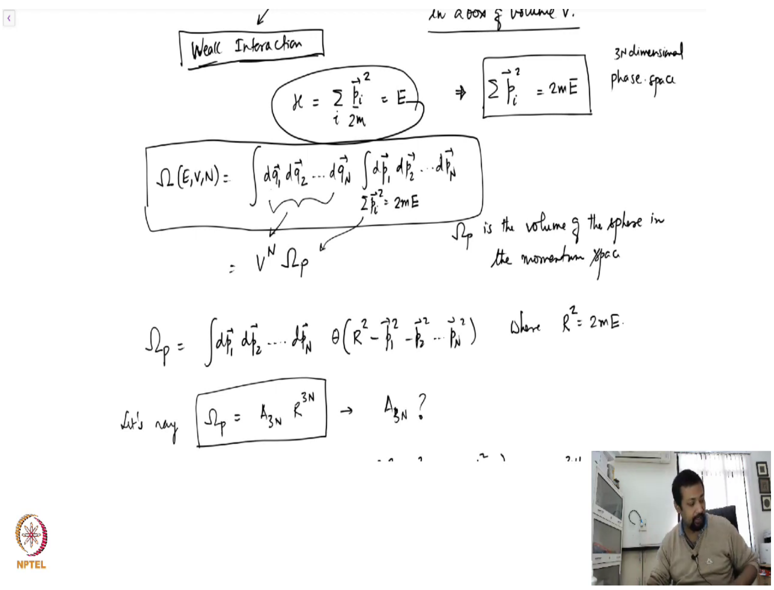

So, the Hamiltonian of this system is sum over I p i square over twice m right. And this is equal to E which means p i square is equal to twice m E. So, if you are looking at this in the phase space, then it is a hypersphere in 3N dimensional phase space. Note that the Hamiltonian does not have any interaction, and therefore, the coordinate is not there. So, the sole representation of the phase space is your momentum right.

So, now, I want to determine the total number of microstates. And the total number of microstates is the volume which is contained within the phase space. So, that that is going to be d q 1 d q 2 all the way up to d q n integral d p 1 d p 2 all the way up to d p n. But now this also has to be satisfied right.

So, that the volume of this happens over the region of r where well let us say over the volume where sum over p i square is equal to twice m E correct. q 1 is allowed to take a volume V. So, therefore, this part is going to be V. And this part we will denote as omega p, where omega p is the volume of the hypersphere in the momentum space right.

So, we just have to figure out the volume of this. So, omega p is going to be integral d p 1 d p 2 all the way up to d p n. And you have a theta function R square minus p 1 square p 2 square p N square, where R square is equal to twice m E right. So, this is the volume that we have to calculate.

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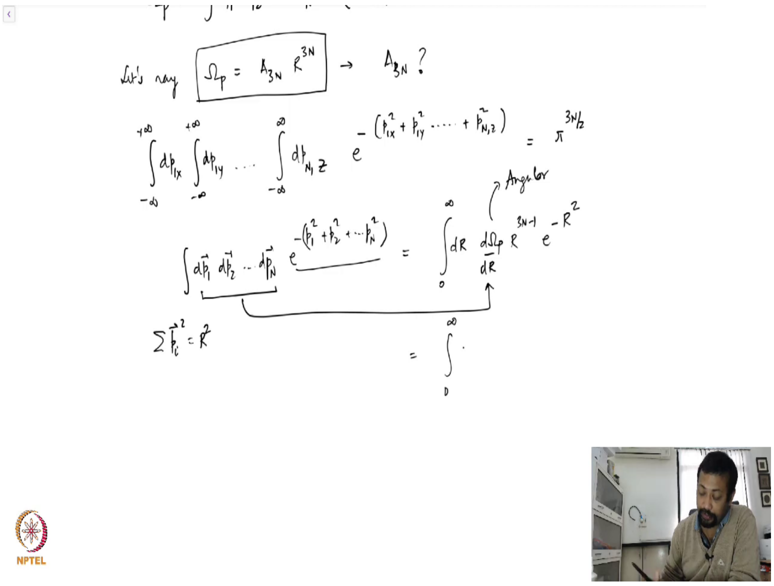

Let us say that omega p is going to be A 3 N r to the power 3 N right. So, this is what we start off with. We now have to figure out what is A 3 N. For this let us consider the integral minus infinity to plus infinity d p 1 x d p 1 y d p 3 N comma z, sorry this is d p N comma z e to the power minus p 1 x square p 1 y square so on and so forth, all the way up to p N set square right.

Now, this integral I know, each of this is a Gaussian integral, and therefore, this integral is pi to the power 3 N by 2 right. But if you look at this integral carefully, then I can recast this integral in this form for in the since it is spherical symmetry, so therefore, I can write down the same integral as integration of d p 1 d p 2 d p N e to the power minus p 1 square p 2 square p N square which I write as d R d omega p dR R to the power 3 N minus 1 right 0 to infinity.

So, this is typically the volume of e to the power minus R square, because I have sum over p i square is equal to R square. Since this part is spherically symmetric I take this measure and represent it in spherical polar coordinate system. This is the part angular part that you have. And using the form of this, I have 0 to infinity. I am sorry; this is just not going to be R to the power 3 N minus 1, this is wrong. So, it has to be e to the power minus r square that is all right.

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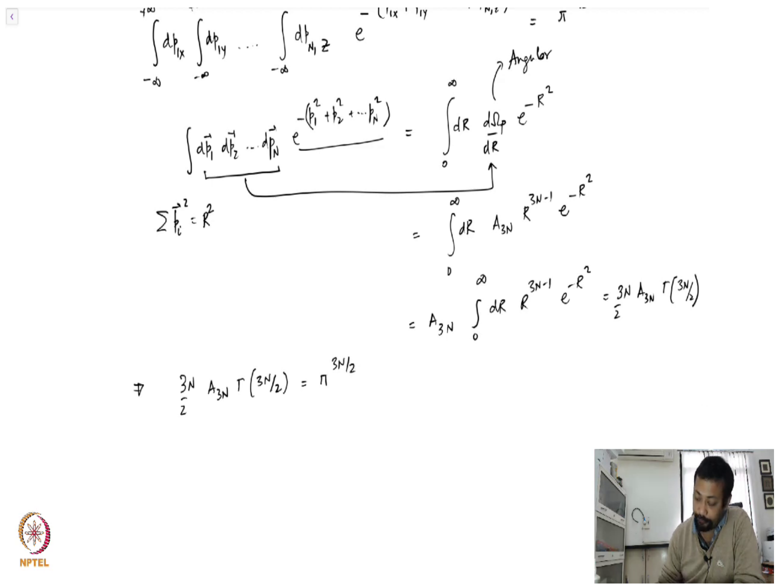

Now, if I use this, d omega d p, then this becomes A 3 N R to the power 3 N minus R e to the power minus r square correct. So, that this integral is a 3 N 0 to infinity dR R to the power 3 N minus 1 e to the power minus R square. And this is going to be a gamma function, it is going to be 3 by 2 N A 3 N gamma of 3 N by 2. This implies that 3 N by 2 A 3 N gamma 3 N by 2 is pi to the power 3 N by 2.

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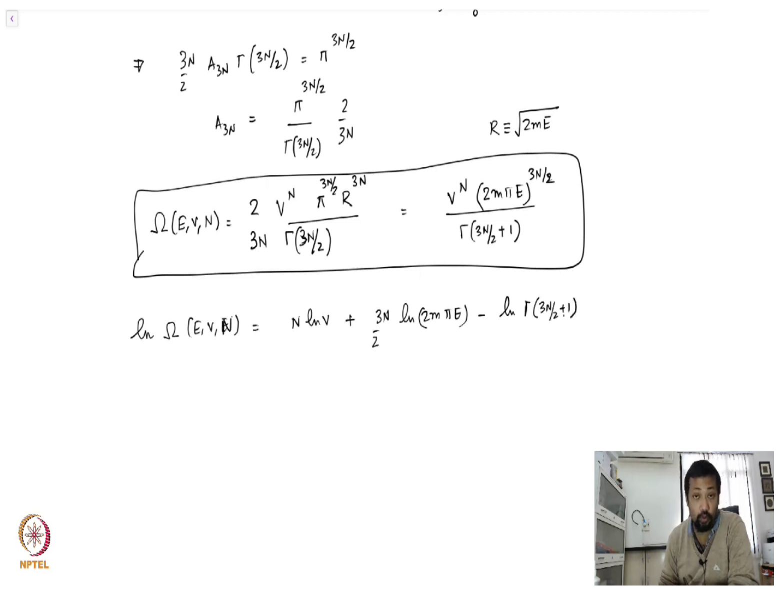

So, that I can immediately write A of 3 N as pi to the power 3 N by 2 gamma 3 N by 2 2 by 3 N right ok. So, therefore, the total number of microstates E, V, N becomes V to the power N there is going to be there has to be an R over here right yeah. So, R to the power 3 N, where R is equivalent to twice m E pi to the power 3 N by 2 gamma 3 N by 2 2 m pi E over 3 N by 2 divided by gamma 3 N by 2 plus 1. So, this is going to be the answer for omega 3 N.

So, if you are if you have not yet followed this, then we will very briefly go we will consider the system of an ideal gas where are N particles which are confined in a box of volume V. I, therefore, the Hamiltonian of the system is given by this which means that in the phase space it is the Hamiltonian does not depend on coordinates. So, in the phase space, it is just a sphere in the hypersphere in the momentum space right.

So, all I have to do is in order to calculate the total number of microstates as we have illustrated, we just calculate the volume that is available between the energy 0 to E. And that volume is essentially given by this where the integration of the momentum should happen over a region where p i square equal to this.

And therefore, once you write down this as each of these coordinates q 1 can have the axis can essentially take values V, I mean they can be over the volume V. And therefore, this part of the integral gives you V to the power N; and this is the part which gives you omega p which is nothing but the volume of the hypersphere in 3 N dimensions that is it. Now, one has to figure out how to calculate this volume.

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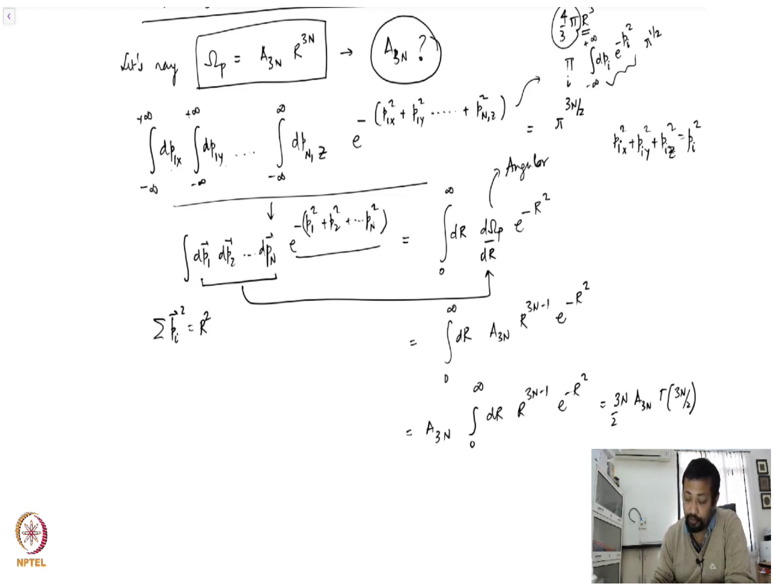

Let us say this volume is A to the A 3 N R to the power N, and this is not very different. Because I know for a 3-dimensional sphere, it is 4 by 3 pi R cube. So, this is the part which is

A 3 N equal to 1 right. If N equal to 1, then if you go back over here, then the determination of A 3 N happens by just looking at this integral. I can separate this integral as each of these integral as product over i integration d p i e to the power minus p i square minus plus infinity.

And this each of this integral is pi to the power half, so that if you take a product of all these integrals, there are 3 N such integrals. And therefore, you will have this to be pi to the power 3 N by 2. I can take now closely since I can write p 1 or let us say p i x square plus p i y square plus p i z square as p i square, I recast this integral in this form because I want to use the spherical the spherical symmetry of the form of the integral.

Since, since the integral is spherically symmetric the measure which was in the Cartesian coordinates you could as you have seen earlier, now it is converted to spherical polar coordinates. And then the rest of it follows immediately, so that you have omega E v N sorry ln of omega E, V, N is N, ln v plus 3 N by 2 ln 2 m pi E minus ln gamma 3 N by 2 plus 1.

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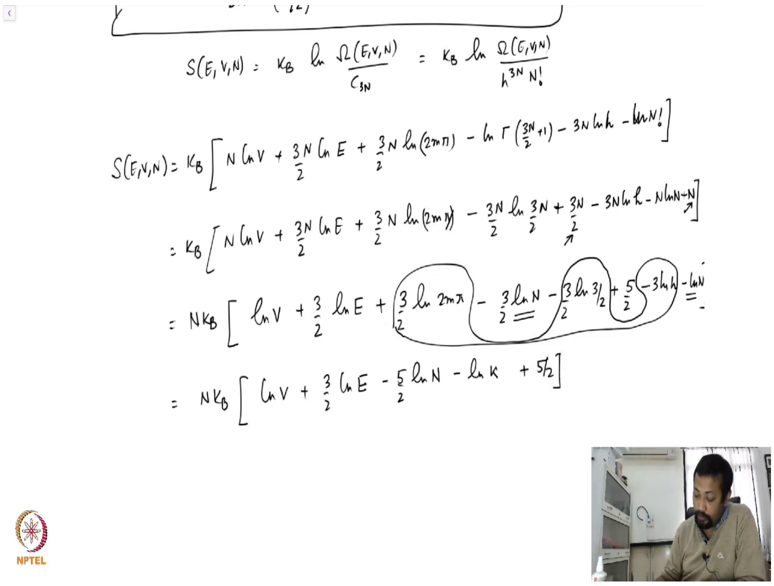

Therefore, the entropy takes the form is K B ln omega E, V, N c 3 N right which in all case is going to be omega E, V, N h to the power 3 N by N factorial because these particles are indistinguishable particles. So, you cannot distinguish between 1 and 2. This gives us let us calculate this N ln v minus plus 3 by 2 N ln E plus 3 by 2 N ln twice m pi minus ln gamma 3 N by 2 plus 1 minus 3 N ln h minus N. So, we will write ln N factorial.

We will next use Stirlimg's approximation to write down the gamma function and the factorial function in the following way. So, the approximation that we are going to use that since N is large enough, this is going to be gamma 3 N by 2 plus 1 is going to be 3 N by 2 factorial, therefore, you have ln 3 N by 2 factorial which is 3 N by 2 ln plus 3 N by 2 minus 3 N ln h minus N ln N plus N.

So, let us take N common, I have N K B outside ln V plus 3 by 2 ln E plus 3 by 2 ln twice m pi minus 3 by 2 ln N minus 3 by 2 ln 3 by 2 plus 3 by 2 there is since I have taken N outside there is going to be plus 3 by 2 here, and there is going to be plus 1 here that gives me 5 by 2 minus 3 ln h minus ln N, so that this is going to give me N K B.

Let us bring together the terms which I am interested in 3 by 2 minus N gives me minus 5 by 2 ln N plus. So, we will just write down minus ln of kappa, where kappa is a constant which you evaluate by plugging in these terms together plus 5 by 2.

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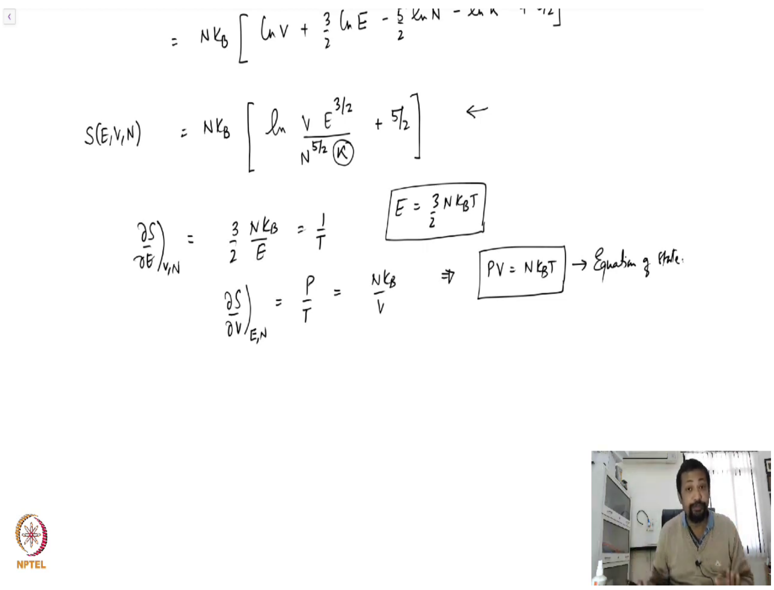

And you see that this expression takes the form ln V E to the power 3 by 2 N to the power 5 by 2 kappa plus 5 by 2, exactly the form of the entropy which we derived for an ideal gas when we are looking at thermodynamics using the Gibbs law humiliation. Except the difference now is I exactly know the form of kappa if I just want to take care of if I just want to look at this put in all these 3 expressions combine them into a simple one, I exactly know the form of kappa.

So, once again statistical mechanics first of all the approach that we have taken gives you the correct expression for the entropy for an ideal gas – number-1. The second point is this quantity kappa is exactly known. So, del S del E V and N held constant is just 3 by 2 N K B by E and this is equal to T, so that for an ideal gas you have 3 by 2 N K B T in accordance with what we did earlier.

Second del S del V E and N held constant is P by T which is going to be N K B over v which implies P V is equal to N K B T. This is also the equation of state which you are very familiar with. So, our expression for entropy, the way we calculate it by calculating the microstates contained within the volume gives us the correct equation of states the correct entropy that we have seen in thermodynamics both E equal to 3 by 2.

And K B T as well as P V is equal to N K B t are experimentally verifiable and they have been verified also. Therefore, our microscopic theory stands a very good, stands on a firm footing.

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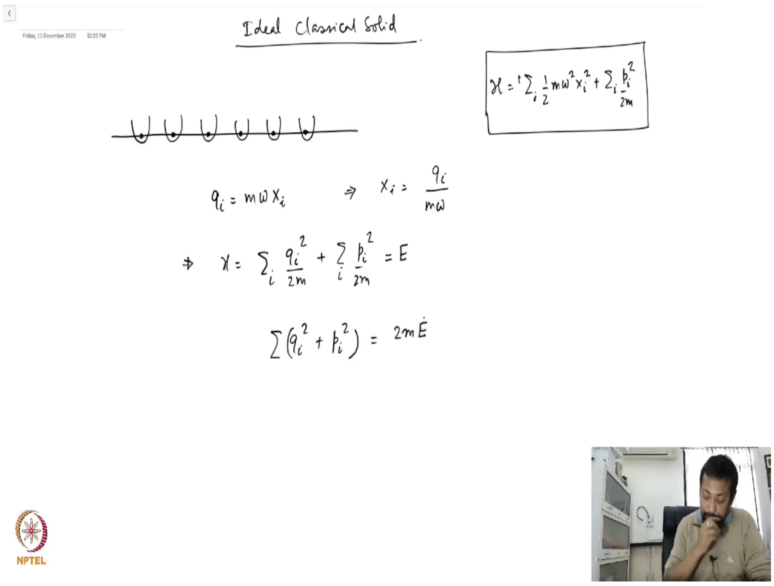

We now want to look at a different classical system which models which is a very, very simple model for a solid. So, we want to look at an ideal classical solid. And the model is very very simple that I have a one-dimensional lattice where at each of these lattice points I have atoms which are sitting, and I have a harmonic potential at each of these lattice points right.

So, that the Hamiltonian of the system is half, well, half m omega square x i square plus sum over i p i square over twice m right. Now, I want to apply this system is isolated, and therefore, I want to apply our microcanonical ensemble to the system, and try to figure out the entropy of the system correct ok.

First node that if I substitute q i is equal to m omega x i this would imply that x i is q i over m omega which means that the Hamiltonian now takes the form sum over I q y square over twice m plus sum over i p i square over twice m. And this is going to be a constant energy. So, in the phase space, then this equation q i square p i square is equal to twice m E defines a 6 N dimensional sphere. Of course, the picture that I have drawn over here is purely one-dimensional.

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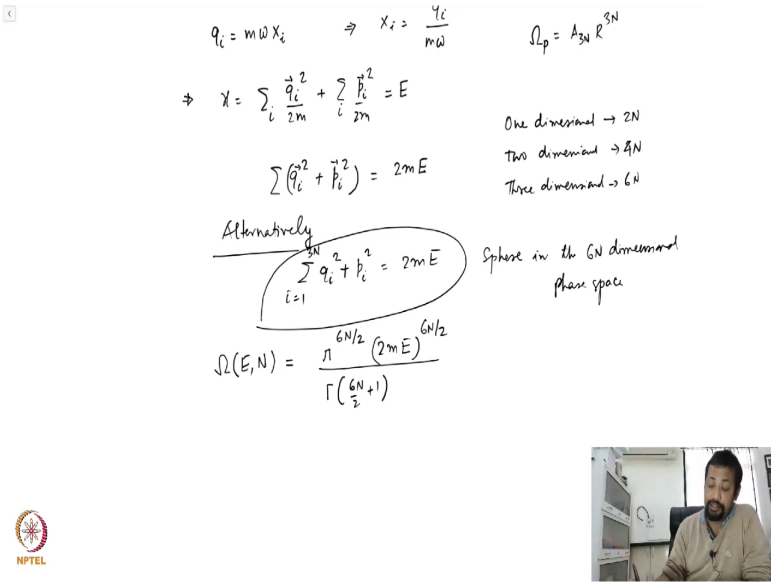

Since, if you have a one-dimensional system, then essentially you have a two-dimensional hyperspheres N coordinates and N momenta one-dimensional you have 2 N degrees of freedom, therefore, this is the dimension of phase space; two-dimensional this goes to 4 N. And 3-dimensional this goes to 6 N.

So, if you are thinking about this in 6-dimensional, one has to be careful in putting a vector sign in all of these, right. Alternatively, you can say that i runs from 1 to 3 N; alternatively if you want to avoid such confusions, you can simply say q i square plus p i square is equal to twice m E, where i is equal to 1 to 3N that is all good.

Now, you see this is a sphere in the 6 N dimensional phase space. And I know the volume in a 6 N dimension of a 3 N dimensional hypersphere we just calculated this for an ideal gas. So, our total number of microstates E and N is going to be the volume of this hyper 6 N dimensional hypersphere.

So that is 6 N by 2 twice m E 6 N by 2 divided by gamma 6 N by 2 plus 1 right. You this is just we had earlier that omega p the volume was A 3 N R to the power 3 N. Here of course, the dimension is 6 N. So, this becomes a 6 N R to the power 6 N, and this is the expression that you should have.

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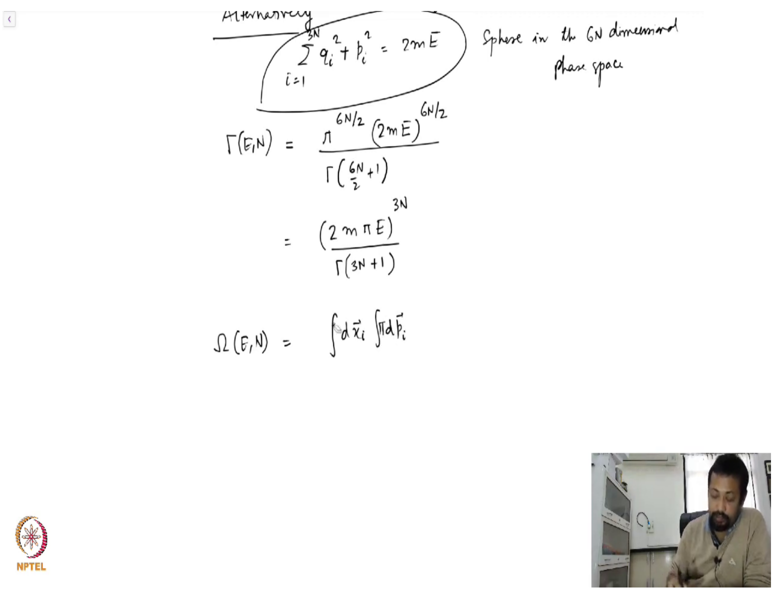

So, one can simplify this in writing twice m pi E 3 N divided by gamma 3 N plus 1 right. So, this is clearly the hypersphere when you consider in this coordinates q i and p i. But we started of this real space coordinate x i and the momenta p i.

So, for us, if we will just change this maybe we change this over here, we write this as gamma E comma N. So, if I want to calculate omega E comma N, the proper calculation is going to be d x i d p i with the product ok. Let us just write this carefully.

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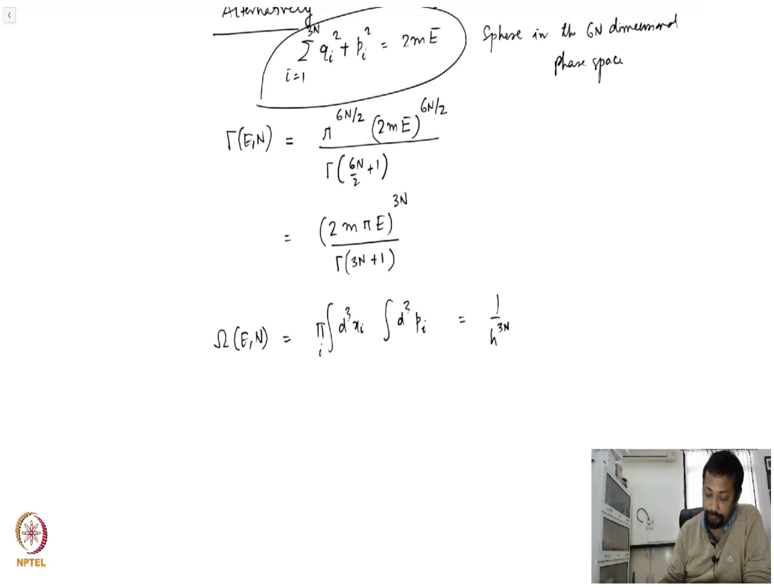

So, d cube x i d cube p i and a product over this integrals right. And this is 1 over h to the power 3 N. Well, the 1 over h to the power 3 N we will introduce later on, but right now we just want to write down x i is q over.

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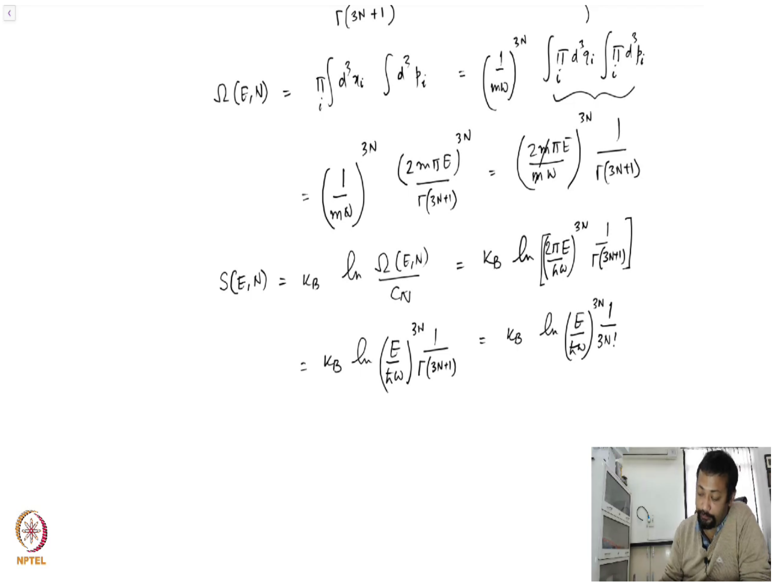

So, this becomes 1 over omega raised to the power 3 N integration product over i d cube q i product over i d cube p i. So, this only tells you that these are in 3 dimension right, the measure itself tells you. But this we just calculated this we calculated over here as this. So, this becomes our actual total number of microstates is twice m pi E over 3 N divided by gamma 3 N plus 1.

I can simplify this twice m pi E over m omega raised to the power 3 N 1 over gamma 3 N plus 1. Well, one can check this out very nicely and then essentially you have S the entropy of this system is K B ln omega E, N the total number of microstates divided by the constant, to make it dimensionless which I have is 1 over h to the power 3 N. The 1 over h to the power 3 N I can plug it in over here, in writing E 2 pi E by h omega raised to the power 3 N 1 over gamma 3 N plus 1 right.

Now, it is in a very elegant and simple form. So, I have K B ln E over h bar omega raised to the power 3 N 1 over gamma 3 N plus 1. For large enough N I can approximate the gamma function again by a factorial which becomes K B ln E over h bar omega raised to the power 3 N 1 over 3 N factorial right.

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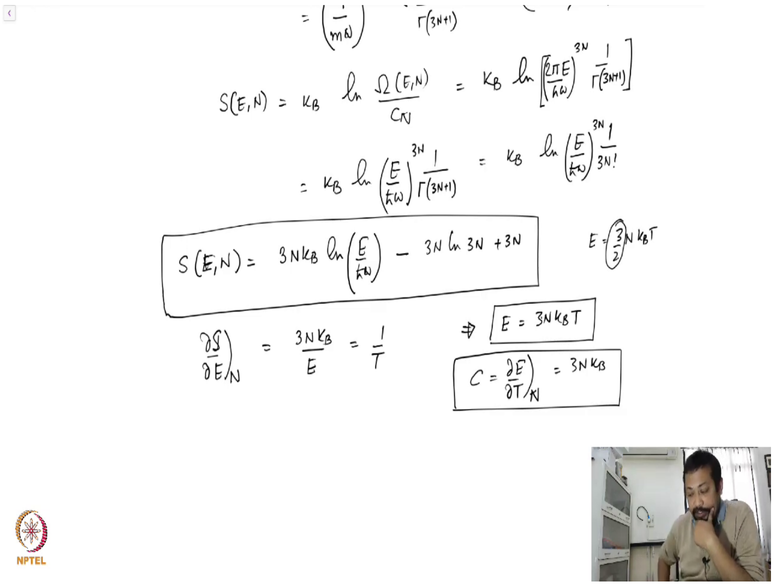

So, S over E comma N, let us now expand this is 3 N K B ln E over h bar omega, this is dimensionless, minus 3 N ln 3 N plus 3 n. So, this is the entropy of your ideal solid. del s del t sorry del s del E N held constant there is no volume which appears over here because your Hamiltonian itself now depends on the coordinates it is just 3 N K B over E and is equal to 1 by T, which implies that the energy is 3 N K B T.

The specific heat which is del E del T N constant is just 3 N K B. And this relation that you have is called the Dulong-Petit law. This is the energy of the system as a function of temperature. Now, surprisingly here for an ideal gas we had there is a difference. And for an ideal gas we had 3 by 2 N K B T; on the other hand, here I have 3 N K B T.

And the reason behind that lies in the Hamiltonian. In the ideal gas, the Hamiltonian did not have this contribution did not have the contribution from the coordinates. It only had the contribution from the momenta. So, this extra degree of freedom actually contributes additional 3 by 2 N K B T. So, that the total energy goes to 3 N K B T right.

So, with this discussion, we are going to conclude our micro canonical ensemble, and then we are going to move onto canonical ensemble.