Advanced Thermodynamics and Molecular Simulations
Prof. Prateek Kumar Jha
Department of Chemical Engineering
Indian Institute of Technology-Roorkee

Lecture - 20
Summary of Thermodynamic Ensembles; Partition Function of an Ideal Gas

Hello, all of you. In this lecture, we will summarize the discussion we were having on the thermodynamic ensembles and basically go over the formula for all the ensembles once again. And then I will talk about how to get the partition function in terms of what is known as a molecular partition function and we give an example of an ideal gas for which we can exactly evaluate the partition function.

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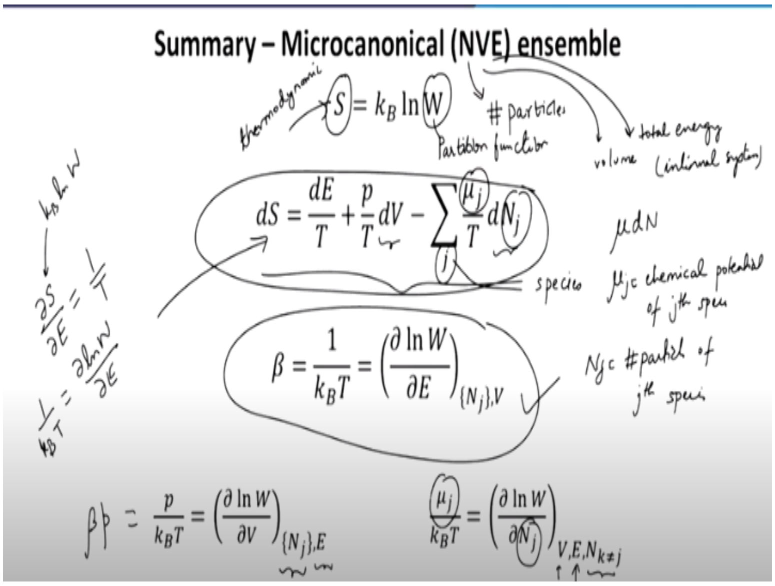

Summary – Microcanonical (NVE) ensemble

$$S = k_B \ln W$$

$$dS = \frac{dE}{T} + \frac{p}{T}dV - \sum_j \frac{\mu_j}{T} dN_j$$

$$\beta = \frac{1}{k_B T} = \left(\frac{\partial \ln W}{\partial E}\right)_{\{N_j\},V}$$

$$\frac{p}{k_B T} = \left(\frac{\partial \ln W}{\partial V}\right)_{\{N_j\},E} \qquad \frac{\mu_j}{k_B T} = \left(\frac{\partial \ln W}{\partial N_j}\right)_{V,E,N_{k\neq j}}$$

So essentially what we have done so far we have been doing different ensembles. The simplest is ensemble is the micro canonical ensemble in which the number of particles, the volume and the total energy that is the internal energy of the system are the control variables. And for this case, the entropy becomes the thermodynamic function which is written as a function of the number of ways of distribution essentially speaking W becomes the partition function although we did not explicitly state that for the case of a micro canonical ensemble.

$$S = k_B \ln W$$

So if I know W I can find S and once I know S I can find all the other variables using the differential form. So keep in mind that while I was doing it, I was keeping it for just one component and therefore we only had a μdN appearing there. If I want to generalize it for multiple component the idea remains the same. We will have a sum over all the species and then we will have chemical potential of the jth species and Nj is the number of particles of jth species.

So now the first thing, what we can do is define a quantity called β that is 1 over k_B T. We argued that we can justify the β as the definition of temperature by saying that, let us say if you have two systems in close contact, and then you have ensemble of such systems, then there must be something common between the systems, which was the Lagrangian multiplier and the Lagrangian multiplier, we defined as-

$$\beta = \frac{1}{k_B T}$$

We also looked at the link between the equation that we have discussed earlier that simply come from the first law of thermodynamics with the equation we derived on the basis of the partition function. And using that as well, we said that the Lagrange multiplier β must be equal to 1 over k_BT and then, the remaining process is quite straightforward there is different ways to look at it.

Let us say for example, I could start with this particular expression and say that the temperature for example, can be defined as doh S by doh E is equal to 1 over temperature. And since we have said that S is equal to k B ln W, so I can replace this with k B ln W. And therefore, I can say that 1 over k B T is doh ln W by doh E. So I am taking the first derivative of dS with respect to dE that is the first result we have. Now we have two more terms appearing here that is dV and dN j. So I can also take derivative of the ln of W, that is the partition function in this case with respect to volume and the number of molecule-

$$\frac{\partial S}{\partial E} = \frac{1}{T}$$

$$\frac{1}{k_B T} = \frac{\partial lnW}{\partial E}$$

$$dS = \frac{dE}{T} + \frac{p}{T}dV - \sum_j \frac{\mu_j}{T} dN_j$$

And naturally what we get is the pressure and chemical potential. So we wrote this as-

$$\beta p = \frac{p}{k_B T} = \left(\frac{\partial \ln W}{\partial V}\right)_{\{N_j\},E}$$

If I take a derivative with respect to volume, it is a partial derivative. So meaning that the number of molecules of all the species or number of particles are held constant. The energy is held constant. In that case, we get the pressure. I can also take derivative with respect to the number of particles of one of the species keeping the volume fixed, energy fixed and number of particles of all the other species fixed that I represent by N_k not equal to j and that will give me the chemical potential.

$$\frac{\mu_j}{k_B T} = \left(\frac{\partial \ln W}{\partial N_j}\right)_{V,E,N_k \neq j}$$

So this is another way of looking at the result comparing the differential form that we already had from the first law of thermodynamics, with just one change that I replaced the thermodynamic function as the function of the partition function and therefore, the idea is that we can evaluate the properties as a function of the partition function.

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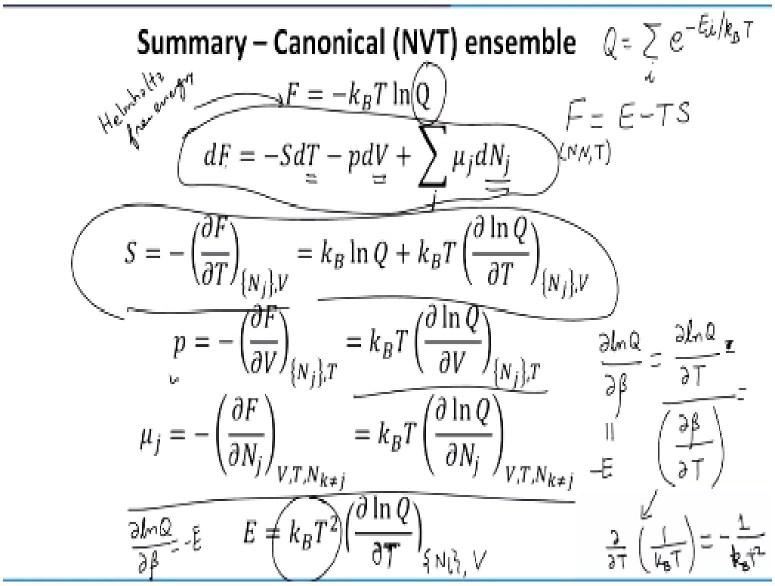

Summary – Canonical (NVT) ensemble $Q = \sum_i e^{-E_i/k_B T}$

Helmholtz free energy

$$F = -k_B T \ln Q$$

$$F = E - TS$$

$$dF = -SdT - pdV + \sum_j \mu_j dN_j \quad (N,V,T)$$

$$S = -\left(\frac{\partial F}{\partial T}\right)_{\{N_j\},V} = k_B \ln Q + k_B T \left(\frac{\partial \ln Q}{\partial T}\right)_{\{N_j\},V}$$

$$p = -\left(\frac{\partial F}{\partial V}\right)_{\{N_j\},T} = k_B T \left(\frac{\partial \ln Q}{\partial V}\right)_{\{N_j\},T}$$

$$\mu_j = -\left(\frac{\partial F}{\partial N_j}\right)_{V,T,N_{k\neq j}} = k_B T \left(\frac{\partial \ln Q}{\partial N_j}\right)_{V,T,N_{k\neq j}}$$

$$\frac{\partial \ln Q}{\partial \beta} = \frac{\frac{\partial \ln Q}{\partial T}}{\left(\frac{\partial \beta}{\partial T}\right)} = -E$$

$$\frac{\partial}{\partial T}\left(\frac{1}{k_B T}\right) = -\frac{1}{k_B T^2}$$

$$\frac{\partial \ln Q}{\partial \beta} = -E \qquad E = k_B T^2 \left(\frac{\partial \ln Q}{\partial T}\right)_{\{N_i\},V}$$

Now if I go to the canonical ensemble, then all that is changed is the expression of the partition function Q is no longer the number of ways to be precise Q is-

$$Q = \sum_i e^{-\frac{E_i}{k_B T}}$$

And now using this Q, I can define the thermodynamic functions. In earlier case S was-

$$S = k_B \ln W$$

where W was the partition function.

In this case, the thermodynamic function is my Helmholtz free energy which is still a function of the partition function, but now we have the canonical partition function i.e.-

$$F = -k_B T \ln Q$$

Again, we have done this differential form. This we have done before even the particle function thing i.e.-

$$dF = -SdT - pdV + \sum_j \mu_j dN_j$$

This comes from again the first law of thermodynamics, where we apply Legendre transformation to go from energy to f. So essentially F is E - TS. So we did a Legendre transformation and we got f that is a function of N, V and T.

And then just like what we did in the earlier case, we can take the derivative or the partial derivative of (f) with respect to temperature or volume or the number of molecule. If I do the first one, I get the entropy and again I can write entropy as a function of the partition function, because I can write (f) as a function of the partition function.

$$S = -\left(\frac{\partial F}{\partial T}\right) = k_B \ln Q + k_B T \left(\frac{\partial \ln Q}{\partial T}\right)_{\{N_j\},V}$$

Similarly, if I take derivative with respect to the volume, I get my pressure. Again I can write it as a function of the canonical partition function.

$$p = -\left(\frac{\partial F}{\partial V}\right)_{(\{N_j\},T\}} = k_B T \left(\frac{\partial \ln Q}{\partial V}\right)_{\{N_j\},T}$$

And finally, I can also get the chemical potential if I take a derivative with respect to N_j.

$$\mu_j = -\left(\frac{\partial F}{\partial N_j}\right)_{(V,T,N_k \neq j\}} = k_B T \left(\frac{\partial \ln Q}{\partial N_j}\right)_{V,T,N_k \neq j}$$

And if I take a derivative with respect to the temperature of the ln Q and multiply with k_B T square we have derived this that is at constant number of molecules and the volume what we have is the average energy of the system-

$$\frac{\partial \ln Q}{\partial \beta} = -\bar{E}$$

So if I put beta is equal to 1 by k_B T I can write essentially as-

$$\frac{\partial \ln Q}{\partial \beta} = \frac{\frac{\partial \ln Q}{\partial T}}{\frac{\partial \beta}{\partial T}} = \frac{\partial}{\partial T}\left(\frac{1}{k_B T}\right) = -\frac{1}{k_B T^2}$$

And this quantity, this entire quantity is equal to my average energy E with a minus sign. So therefore, we get-

$$E = k_B T^2 \left(\frac{\partial \ln Q}{\partial T}\right)_{\{N_j\},V}$$

So all the derivation that we have done, if I am doing in terms of βI can always convert in terms of derivative with respect to the temperature in the same way we simply divide with doh beta by dou T and we can write the expression in terms of temperature. This is how they are typically represented or typically useful because we are interested in the temperature.

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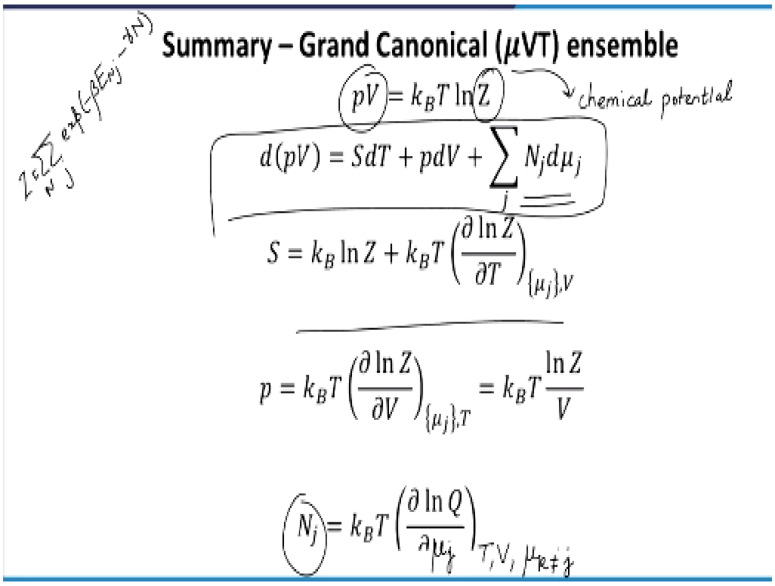

Summary – Grand Canonical (μVT) ensemble

$Z = \sum_N \sum_j \exp(-\beta E_{Nj} - \gamma N)$

$$pV = k_B T \ln Z$$

chemical potential

$$d(pV) = SdT + pdV + \sum_j N_j d\mu_j$$

$$S = k_B \ln Z + k_B T \left(\frac{\partial \ln Z}{\partial T}\right)_{\{\mu_j\},V}$$

$$p = k_B T \left(\frac{\partial \ln Z}{\partial V}\right)_{\{\mu_j\},T} = k_B T \frac{\ln Z}{V}$$

$$N_j = k_B T \left(\frac{\partial \ln Q}{\partial \mu_j}\right)_{T,V,\mu_{k \neq j}}$$

Now if I go to the grand canonical ensemble, now the number of molecules are also not the control variables. In this case, we are dealing with an open system where the number of particles can change. So in that case, instead of the number, the chemical potential becomes the control variable. And the thermodynamic function as we derived in this case is-

$$pV = k_B T \ln Z$$

and Z is the grand canonical partition function that I can also write as a function of the canonical partition function. So Z essentially was-

$$Z = \sum_N \sum_j \exp(-\beta E_{Nj} - \gamma N)$$

And we said that γ is related to the chemical potential. We can generalize this again for multicomponent by doing the summation over j. And then we can also get the differential form in the same way that we have gotten earlier. Keep in mind in the last term, we have N_j d μj.

$$d(pV) = SdT + pdV + \sum_j N_j d\mu_j$$

Now again I can define the entropy as a function of the partition function for the grand canonical ensemble.

$$S = k_B \ln Z + k_B T \left(\frac{\partial \ln Z}{\partial T}\right)_{\mu_j, V}$$

And I can find the properties by taking a derivative of the partition function in the same way that we have been doing-

$$p = k_B T \left(\frac{\partial \ln Z}{\partial V}\right)_{\{\mu_j\}, T} = k_B T \frac{\ln Z}{V}$$

In this case, we can also find the average number of molecules of every species as a derivative of ln Q with respect to the mu j or the chemical potential keeping the temperature, volume and chemical potential of all the other species being held constant.

$$N_j = k_B T \left(\frac{\partial \ln Q}{\partial \mu_j}\right)_{T, V, \mu_{k \neq j}}$$

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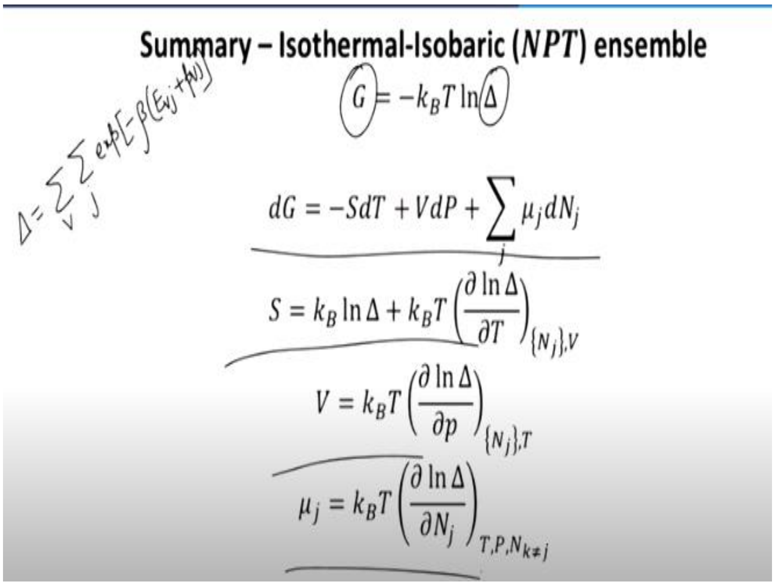

Summary – Isothermal-Isobaric (NPT) ensemble

$$\Delta = \sum_V \sum_j \exp[-\beta(E_{Vj} + pV)]$$

$$G = -k_B T \ln \Delta$$

$$dG = -SdT + VdP + \sum_j \mu_j dN_j$$

$$S = k_B \ln \Delta + k_B T \left(\frac{\partial \ln \Delta}{\partial T}\right)_{\{N_j\}, V}$$

$$V = k_B T \left(\frac{\partial \ln \Delta}{\partial p}\right)_{\{N_j\}, T}$$

$$\mu_j = k_B T \left(\frac{\partial \ln \Delta}{\partial N_j}\right)_{T, P, N_{k \neq j}}$$

So finally, we have also discussed the isothermal isobaric ensemble. Now we have a partition function that is again new i.e.-

$$G = -k_B T \ln \Delta$$

And that now depends on the pressure and we found that Δ was-

$$\Delta = \sum_{V}\sum_{j} \exp\left[-\beta\left(E_{vj} + pV\right)\right]$$

And now again, we have a differential form. The thermodynamic function in this case is the Gibbs free energy-

$$dG = -SdT + VdP + \sum_{j} \mu_j dN_j$$

I can again write entropy as a function of the partition function.

$$S = k_B \ln \Delta + k_B T \left(\frac{\partial \ln \Delta}{\partial T}\right)_{\{N_j\},V}$$

I can again write the volume and the chemical potential as a function of partition function as-

$$V = k_B T \left(\frac{\partial \ln \Delta}{\partial p}\right)_{\{N_j\},T}$$

$$\mu_j = k_B T \left(\frac{\partial \ln \Delta}{\partial N_j}\right)_{T,P,N_{k \neq j}}$$

So the basic math remains the same. It may seem involved, but the procedure that we have done is pretty much the same no matter what we are doing but the partition function changes as we change the ensemble. So now let us come to the point on of how exactly we get the partition function, right. If I know the partition function, and we have shown also for the ideal gas, and for the Van der Walls gas, that if I know the partition function, I can find the properties but knowing the partition function itself is something that we have not discussed so far.

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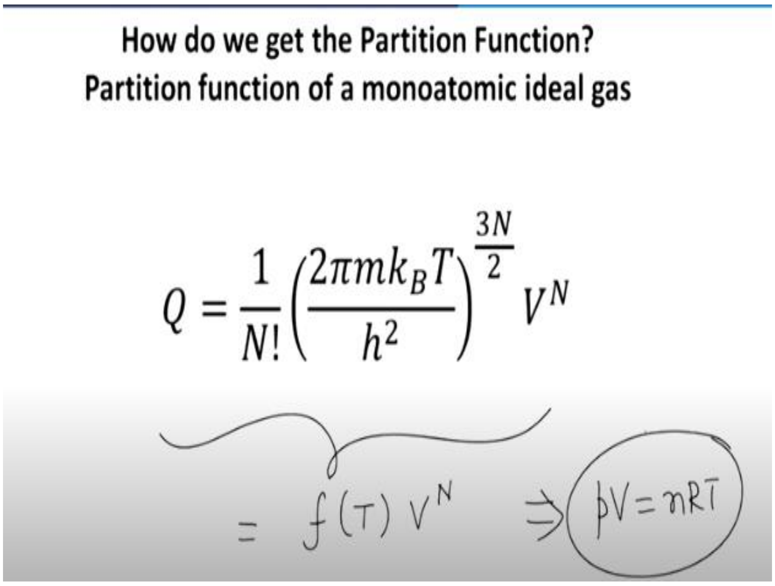

How do we get the Partition Function?
Partition function of a monoatomic ideal gas

$$Q = \underbrace{\frac{1}{N!}\left(\frac{2\pi m k_B T}{h^2}\right)^{\frac{3N}{2}}} V^N$$

$$= f(T)\, V^N \Rightarrow \boxed{pV = nRT}$$

So we started with-

$$Q = \frac{1}{N!}\left(\frac{2\pi m k_B T}{h^2}\right)^{\frac{3N}{2}} V^N$$

And we said that I can write this as some function-

$$Q = f(T)V^N$$

And using that we established that we can get the ideal gas law-

$$pV = nRT$$

And the question is, how do we get this Q? How do we derive this expression of Q? So the answer to this lies in the idea of a molecular partition function. So in this lecture, I will try to get to how can we represent the partition function in terms of the molecular partition function.

Now as soon as we talk about a molecular partition function, the concept itself is a bit confusing, because as we started the discussion of thermodynamics, I said that we are talking about a large number of molecules. So whenever we are talking about any thermodynamic behavior, that does not apply to one molecule, it applies to a collection of molecules only then the thermodynamics start making sense. For example, I cannot define entropy of an isolated molecule in bulk only when you have the bulk comprised of a large number of molecule we can define the entropy. The disorder will come into existence only when we have a large number of molecules.

Similarly, all the notion of the laws of thermodynamics implicitly assume that we have a large number of molecules. Nonetheless, theoretically there is a linkage that can be exploited between the quantum mechanics, how we define energy of the quantum systems and how can we extend that to the thermodynamics and we have already used this idea earlier as well. For example, when I first defined the entropy, I said let us look at how can we distribute certain quanta of energy into so many particles and in there we are implicitly using the idea of discrete energy levels that come from quantum mechanics.

So let us go back to that kind of a discussion and try to justify the meaning of a molecular partition function and then from there, we can see how exactly we can derive the partition function of a monatomic ideal gas.

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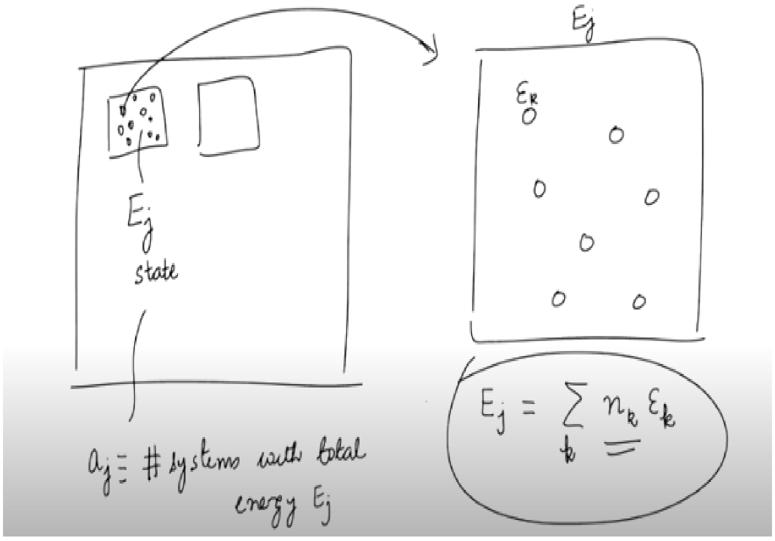

So the idea begins from here that until so far, I have been talking about the energy of a system that is already comprised of a large number of molecules and the partition function is essentially written in terms of these energies, right. If I look at the canonical partition function or the grand canonical partition function, for the micro canonical ensemble this energy is held constant but for all the other ensembles that we have discussed, this energy is a variable and therefore the partition function was in terms of this energy.

But now if I look at any of these particular systems, there is another energy that we have discussed earlier that is the energy of the molecules. So when we say that the system has an energy Ej what essentially we are saying is that this energy Ej is distributed into the molecules or particles comprising the system.

So therefore, we have earlier used the notation some ϵ_k for those energies of the molecules in the system. So let us say for example, if I talk about E_j of a particular state right here that is written as-

$$E_j = \sum_k n_k \, \mathrm{E}_k$$

So therefore, we have pretty much gone from like a molecular level distribution of quanta that we have discussed earlier to a system level description of the total energy of the system that already comprises of the molecular level distribution, right. But nonetheless, the idea was very similar the way it was transmitted from here to there. We still had a constraint of energy conservation that can pretty much be written also for this particular case. This is the equation that must be satisfied for the system. We can define total energy of a system and therefore, we can talk in terms of energy of the molecules.

So let us say for example, I look at my canonical partition function now but now in terms of not the energy of a system, but energy of the molecules comprising of the system. In statistical mechanics book, we talk about the idea of micro state and macro state. I am not getting into that semantics in this particular course. But keep in my mind that if you read about those things, it basically refers to this particular picture when we are looking at the distribution of energy in the molecules of a system versus distribution of energy of a systems in the ensemble.

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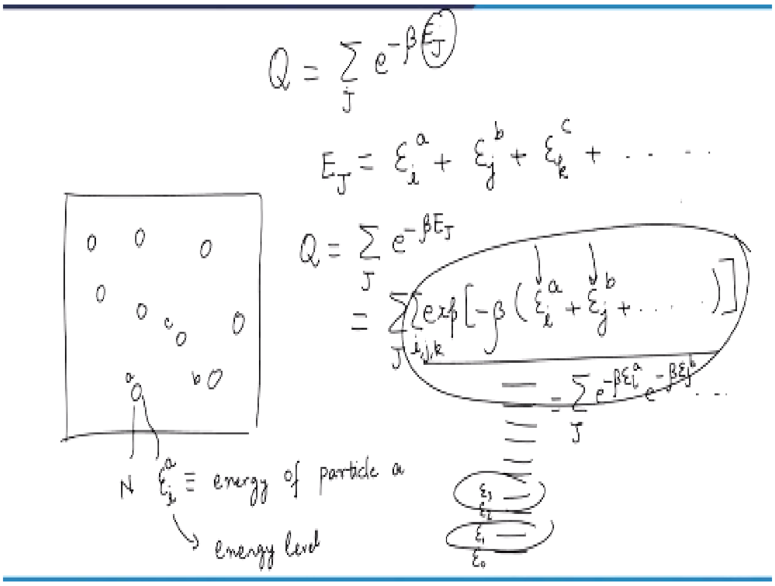

So let us start writing the canonical partition function in terms of these molecular level energy. So this is how we defined it earlier-

$$Q = \sum_j e^{-\beta E_j}$$

But now I want to write this Ej in terms of the molecular energies, right. So what we can write this as is let me for the sake of argument, let us say if you have some N particles, and I will I want to label these particles, so that I can write a partition function of all of them. So let us say I want to label these particles. So let us say they have labeled as something like a, b, c and so on. Now each of these particles a, b and c and so on can have different energy levels, right. So let us say for example, ϵ_i^a represent the energy of particle ‘a’ and that is for a particular system. So i indicate the energy level the particle is in. And ‘a’ is the subscript for the particle.

So let us say for example, if as per the quantum mechanics let us say if there are certain number of discrete energy levels available out there for the molecules or particles then every particle can be in any of these energy levels. So let us say particle a that we have labeled is at a particular energy level, let us say i equal to 3 then the other particle can be at some other energy level, let us say i equal to 1 and so on. So ϵ_i^a indicate the energy of particle a, where i indicate the energy level the particle is in. So then, I can now write Ej as-

$$E_J = \epsilon_i^a + \epsilon_j^b + \epsilon_k^c + \cdots \dots \dots \dots \dots \dots ....$$

So right now we are not even counting the number of particles that have the same energy level. In the earlier case I was telling you Nk particle have this energy level right now I am labeling them separately. So every particle is assumed to be different. We will soon come to the point when they are considered indistinguishable. But let us first label them and say that they have different energy levels.

So clearly, the particle b may not be in the energy level same as a. Let us say it is in some ϵj energy level and let us say the particle c in some energy level k and so on right. Just to keep the indexing right, let me write the energy of the system as the capital subscript. So J refers to the energy levels for the entire system, but capital J refers to energy levels of entire system and small i small j small k refers to the energy level of the molecules under consideration. So therefore, I can then write my Q as-

$$Q = \sum_j e^{-\beta E_j}$$

$$= \sum_j \exp\left[-\beta\left(\epsilon_i^a + \epsilon_j^b + \cdots \dots \dots \dots \dots ..\right)\right]$$

So now what I notice here is that I can break this apart into individual terms, because I can write this as well as summation of j exponential of minus β ϵ_i^a exponential of minus β, ϵ_j^b, and so on.

But now there is a problem in the way we have written it and that problem is that now as soon as I have given an index i j and k and so on there, we are looking at only one particular energy level that is possible for that particular molecule. If I want to count over all the possibilities, then this has to be summed over all the indices i, j and k because partition function refers to sum over the Boltzmann function of all the states but then, within each state I have to sum over the Boltzmann factors of all possible what I refer to as microstates of that particular system.

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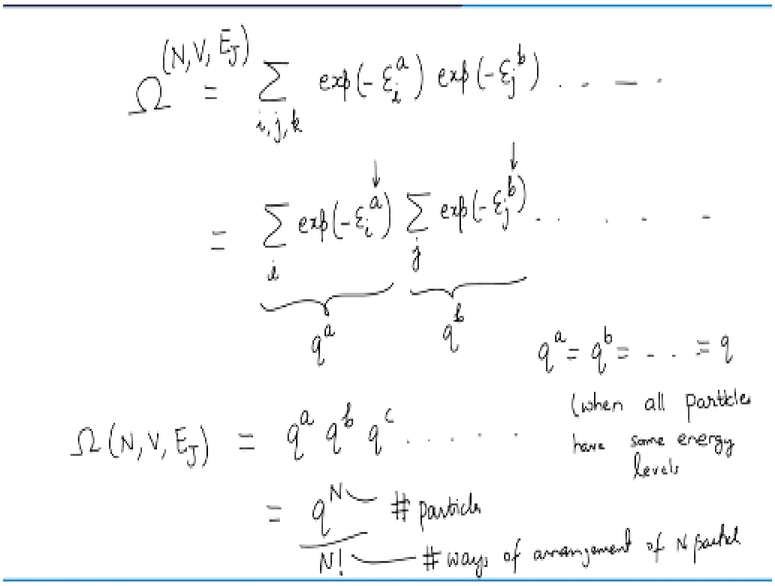

$$\Omega^{(N,V,E_J)} = \sum_{i,j,k} \exp(-\varepsilon_i^a)\exp(-\varepsilon_j^b) \ldots$$

$$= \underbrace{\sum_i \exp(-\varepsilon_i^a)}_{q^a} \underbrace{\sum_j \exp(-\varepsilon_j^b)}_{q^b} \ldots$$

$q^a = q^b = \ldots = q$

(when all particle have same energy levels)

$$\Omega(N,V,E_J) = q^a q^b q^c \ldots$$

$$= \frac{q^N}{N!}$$

N — # particle

$N!$ — # ways of arrangement of N particl

So what it means is that this has to be also summed over i, j, k and so on right. Now it turns out that this need not even be canonical ensemble even if we have micro canonical ensemble where energy of the system is held fixed, even in that case, if I look at the distribution of energy within molecules, they still have a partition function and that partition function comes from the distribution within the system, right. So this quantity is present even if we assume that the energy of the system overall is held constant, right. So therefore, I can define some quantity, let me call it Ω for the time being as-

$$\Omega^{N,V,E_j} = \sum_{i,j,k} \exp(-\epsilon_i^a)\exp\left(-\epsilon_j^b\right) \ldots \ldots \ldots \ldots.$$

So even if it is micro canonical ensemble or a grand canonical ensemble or something else, the key idea is that we are no longer looking at the distribution of energy between systems, but distribution of energy within the system, right. So this is defined for one particular system under consideration. This I can also write as-

$$\Omega^{N,V,E_j} = \sum_i \exp(-\epsilon_i^a) \sum_j \exp -\epsilon_j^b \ldots \ldots \ldots \ldots \ldots.$$

So the other way to say that is we are kind of assuming that the energy level of every particle is kind of independent of the energy level of other. It is like saying that we have so many energy levels available and every particle is free to explore any of the energy level that is an assumption to be precise, but it is good enough for the ideal gas example that we are doing. So then we will have this and so on.

So this tells me, since we have labeled the particle we have one sum each for every particle that we have labelled. Let me call that as the partition function q^a of that particular particle that we have labeled. So it is q^a for a q^b for b and so on. Keep in mind that there is a βin all exponentials here. So therefore, for any given state I can write the partition function as the partition function of the individual molecules.

$$\Omega(N,V,E_j) = q^a q^b q^c \ldots\ldots\ldots\ldots\ldots\ldots$$

Now let us say if I look at a system for which every particle is of the same species. In that case, what do we expect that this molecular partition function are going to be since every particle is of the same species, they are free to explore the same energy levels as every other particle, right. So because discrete energy states depend on the particle under consideration. Let us say if it is a hydrogen atom, then it corresponds to electron being in say, 1 s orbital or 2 s orbital or 3 s orbital and so on those energy levels it can explore is same for every hydrogen atom in the system. If you have a system of hydrogen and oxygen, it is no longer true, but if it is the same atom or same particle or same molecule, in that case, the partition functions are going to be the same.

So therefore, what we can say is $q^a = q^b = q^c$ and so on when all particles have same energy levels. And this I can therefore write as something like q^N. Let us say if I call this quantity q, then q^N when N is the number of particles will give me the partition function of a particular state. If I am interested in the canonical partition function, I still have to sum over all the states but this is corresponding to one particular state of the system. Or in other words, this is the partition function to be precise for a micro canonical ensemble, because for a given system, the number of molecules, the volume and the energy are constant.

Now there is a problem here. The problem is that even though we have labeled the particles as a, b and c, that labeling is something that is not possible in an actual system. In actual system, it is very difficult to find the trajectory of any particular particle because every particular particle is the same. It is not that the particles are colored in the system. The other way to say that is that the particles are indistinguishable and therefore, we need to account for that indistinguishability and the way to do that is we divide this by N factorial, which refers to the number of ways of arrangement of N particles.

$$\Omega(N,V,E_j) = \frac{q^N}{N!}$$

That is to say, if the particles were indeed colored, then there are certain number of ways of arranging them. But, since the particles are not colored, every particle is the same, we need to discount the effect of the arrangement of the particles. And therefore, we are dividing it by N factorial.

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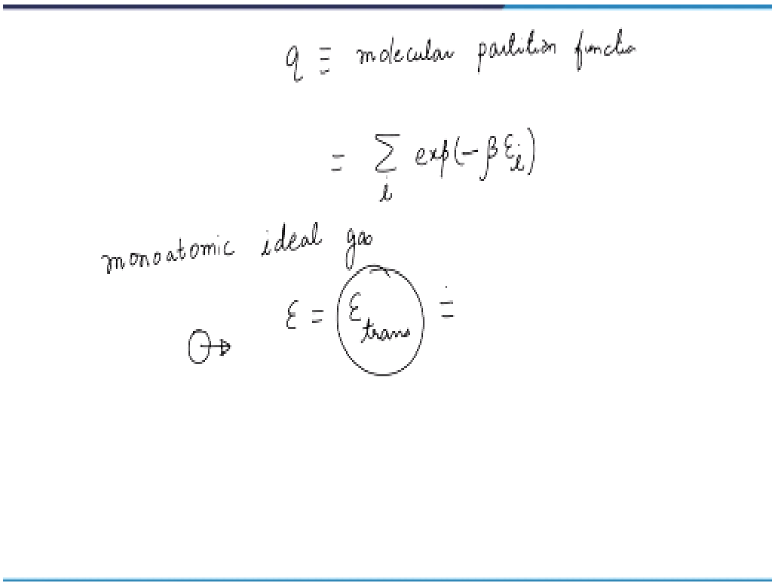

$q \equiv$ molecular partition functio

$= \sum_i exp(-\beta\varepsilon_i)$

monoatomic ideal gas

$\varepsilon = \boxed{\varepsilon_{trans}} =$

So now this q is my molecular partition function which is defined as-

$$q = \sum_i \exp -\beta\epsilon_i$$

where ϵi are the energy levels that are available to the system.

Now let us look at how do we find this ϵi. So that will depend on the particles under consideration. These correspond to the energies of the molecules. So that energy maybe because of as we know it can be because of the kinetic energies or the potential energy. So let us say for example, if you have a monoatomic ideal gas, in that case there is no potential energy because we assume that there are no interactions between particles in the ideal gas. So in that case, the particles may have some motion, and that because of that, it may have some kinetic energy. In fact, this is not the complete answer. There can also be some electronic energies but the effect of that is neglected here assuming that the effect is small in the classical sense.

So in that case, this ϵ will be the translational kinetic energy of the molecules. And that can be determined by solution of the Schrodinger equation or whatever we have and I am not going in details there. But, the key idea is that we can find the translational energy of the molecule and it turns out that this ϵ_{trans} come out to be equal to this quantity to the power 3 by 2 here.

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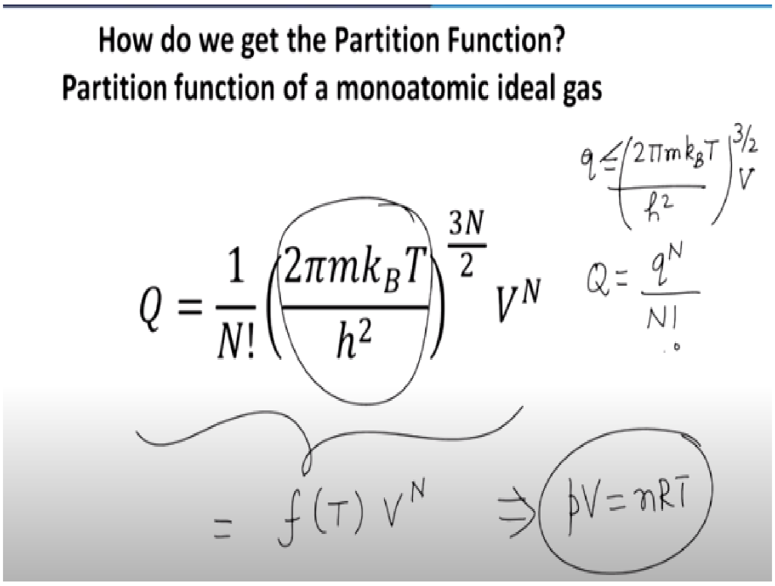

How do we get the Partition Function?

Partition function of a monoatomic ideal gas

$$\underbrace{Q = \frac{1}{N!}\left(\frac{2\pi m k_B T}{h^2}\right)^{\frac{3N}{2}} V^N}$$

$$q = \left(\frac{2\pi m k_B T}{h^2}\right)^{3/2} V$$

$$Q = \frac{q^N}{N!}$$

$$= f(T)\, V^N \Rightarrow \boxed{pV = nRT}$$

So the energy because of the partition function, because of that ϵtrans come out to be-

$$q = \left(\frac{2\pi m k_B T}{h^2}\right)^{\frac{3}{2}}$$

So therefore, what we have is-

$$Q = \frac{q^N}{N!}$$

And therefore, we indeed have a relation between the partition function of the system that is written in terms of the energy states of the systems with a molecular partition function that depends on the energy levels that are being explored by the particular system under consideration.

So with this particular idea, I want to stop the discussion here, we will come back to this argument of how to find the partition function, wherein we will use a simplified model called the lattice model to find the approximate expression of the partition function for a certain case. But for the time being, keep in mind that we have found how to get the thermodynamic variable if I know the partition function.

And we know that the partition function indeed is coming from the partition function or the energies of the molecules of the systems. And for simplified cases, it is possible to evaluate that precisely, and we have given an example for an ideal gas.

So with that I want to stop here. Thank you.