Thermodynamics for Biological Systems:
Classical and Statistical Aspects
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Lecture – 73
Introduction to Computer Simulations

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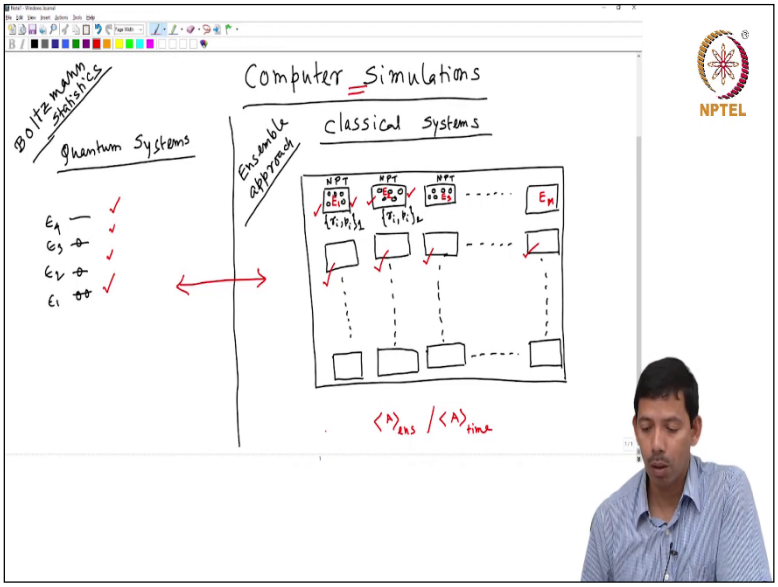

So, today I will be teaching you something called computer simulations. So, you must be wondering how computer simulations would be part of statistical thermodynamics and that is what may I will discuss. So, we started from a small quantum system if you recall the very first few lectures we started from quantum systems and we said that the microstates in a quantum systems are nothing but the energy states and we looked at how the particles are distributed among these energy states epsilon 1, epsilon 1, epsilon 3 and so on so forth.

Then when we came to the biological systems or on liquid systems we said that quantum mechanical approach will not be applicable there because those systems are law systems and there we our approach was classical approach. And we took the classical systems like biological systems are on liquid system. And in classical systems if you recall the ensemble approach due to so this quantum approach was due to Boltzmann and the latter approached the post quantum approach is called the ensemble approach.

And this ensemble approach was this is Boltzmann statistics and then can the ensemble approach proposed by Maxwell Boltzmann and particularly by Gibbs. And in this ensemble approach we

discussed that we in the ensemble of different microstates we have several microstates and so on so forth. So, this microstates are large number very large number of microstates they basically make the ensemble. So, this boxes should be all same dimension it is just that I am drawing without a scale in my hand and therefore they are not looking all the same.

But so basically what I dream is that let us talk about a simple liquid system where I have 5 particles. So, this 5 particles can be distributed differently from box 1, box 2 two box three likewise in all the boxes. So, how the particles are different in these different boxes they are having different XYZ coordinates the positions they are also having different momenta or the velocity. So, here so let us say this is my microstate 1 and here i is basically 1 to 5 since we have 5 particles. So, here also my I goes from 1 to 5 and this is my box 2. So, these states this microstates we call the microstates because they are different from each other.

And their differing from each other by the different positions and velocity of the constituent particles, now and nevertheless each of this box do you have same number of particle which is N equal to 5 here and let us say we are looking at them at the room condition pressure is equal to 1 bar and temperature is equal to the room temperature. So, all of them do have the macroscopic quantity same temperature same pressure same number of particles.

So that macroscopic on do so they are all the same but microscopically they are different because their particle distributions are different and therefore the inter particle interaction would be different. And as I have seen in the previous lecture that when interpreting the interactions are different so these distribution of the particles in each state would have different energy that means if energy of I am sorry I will go back to draw 5 number of particles here. So, I have 5 particles.

And now what I am saying that due to the distribution of the particles here and here are different that energy of the system will also different. So, here let us say my energy is E1 the energy in this box will obviously be different because the particles are distributed differently and therefore their intermolecular or interacting interactions are different because as you saw in the previous class that inter molecular particle interactions depends on this r ij is basically the distance between particle i and j.

So, when they are inter particle distances are different as you can see here hand here it is in the inter particle distances are different their interactions will also be different and therefore their

potential energy will be different and therefore the total energy. So, that the energy in here is E 1 here is E 2 here is E 3 and so on so forth. Some number n and so on. So, therefore in classical systems we have the microstates which are different from each other in their total energy.

So now if you now compare that the quantum system we started do it and the classical systems what we are tackling now there the definition and the concept is exactly the same. Here we looked at the energy states here we are looking at the energy of each of the microstate and the same way so here also our ultimate goal was to get the partition function based on the distribution of the particles among the quantum states and here also will be getting the partition function from averaging over all the energy states.

And where the energy states are now different in their energy from E1 E2 E3 in all so on and so forth, now so as you as you clearly see here that these are microscopic information how the particles are distributed, how the particles have the different velocity from this instant to this instant this instant could be time t1 to t2. So, how the particles are having their microscopic information different as we move along.

And to get those different microstates the microstates having different energy or the different distribution of the particles we are now resorting to computer simulation methods. So, computer simulation method is basically a computer tool which will help us to get these different microstates of our classical systems. So, once we have these microstates available then we can take the ensemble average or over them or you can take the time average about them to get to get our thermodynamic quantity A ensemble average or we can get the time average of the thermodynamic quantity A.

So, in the next part we will be talking about the computer simulation method in particular the molecular dynamics simulation method which will help us to generate the different microstates in an ensemble okay.