ELEMENTS OF MODERN PHYSICS

Prof. Saurabh Basu
Department of Physics
IIT Guwahati

Lec 19: Ensembles, Microstates and Macrostates

So let us get ahead with the study of statistical mechanics. Just wanted to make two points clear. One is that when you study statistical mechanics from a book, it is usually very verbose, which means that A lot of reading needs to be done. A lot of description is given, sometimes through examples or through words.

And you don't find it so attractive to read through all these verbose descriptions. But you have to understand one thing that the author is not present in front of you. So whatever his thoughts are, the way he wants to clarify the concepts and confusions, etc., he has to do it by description. And that's why it often gets verbose, and students find that there's too much to read and feel confused. A little disappointed about that.

But that is part and parcel, and you should read books—there are extremely good books on statistical mechanics. I will just list a few of them. We have a very good book called Pathria. So, Pathria; then there is a good book by Huang. There is a very nice book by James Sethna.

Then there are these McQuarre. I guess this Q has to be a capital Q. And so on. And there are other books as well, but these are some of the books that are very good and they give you a lot of insights into the study of statistical physics. However, each has a distinct way of presentation.

So, my suggestion would be to stick to one book and learn the subject well. And in fact, Pathria is a very good textbook, which is accepted all over. So you may want to have a copy of this and study along with the lecture notes that you have from this course. The second thing is that you would often find me writing on the on the board on this digital board.

And this is to make sure that you do these as I do it in front of you. So you do it on your own and a lot of calculations will get clear when you do these calculations by hand without seeing either the lecture videos or some of the books try to do it themselves. And this is one of the reasons that I do some of the derivations where I I need to speak and give you the steps of derivation, I do that instead of just showing you the slides, which will have lesser effects than what is intended here, alright. So, we will start with ensemble theory.

And the application of statistical mechanics relies on the study of an ensemble of systems and not a single system. In fact, it's often difficult to study the properties of a single system, whereas the properties of similarly prepared—this word is important—similarly prepared systems are possible and often easy to interpret. I'll give you an example that if you are an avid follower of cricket, you would know that somebody talks about either the strike rate or his average scores in an innings for a batter. And that's often taken when he has played at least 20 matches or 50 matches and so on.

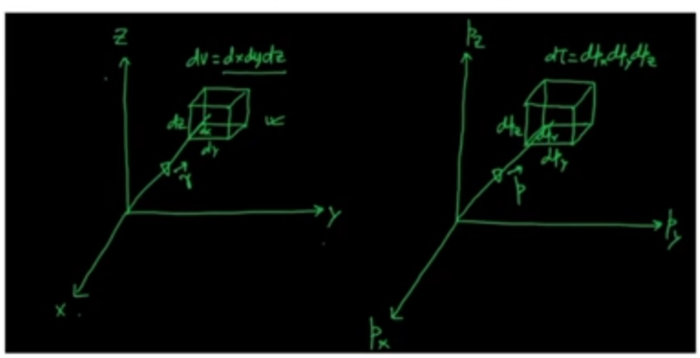
Anything less than that, there is no point in talking about averages. So, a large number of innings or a large number of matches are considered when you talk about averages and so on. So, these are in this technical jargon, they are called as ensembles or these will know what ensembles are. But let me first take you through some of the prerequisites of ensemble theory. One of this is called as phase space and the other is called as a microstates and macrostates.

Phase Space:

We are familiar with configuration space and momentum space.

Configuration space: (x, y, z) with an elementary volume $dxdydz$

Momentum space: (p_x, p_y, p_z) with an elementary volume $dp_x dp_y dp_z$



So, for that, let us take this phase space and in classical mechanics, we are quite familiar with the configuration space and the momentum space. In fact, the configuration space that is, you know, given by x, y, z or r theta phi and so on, they can be solved by solving

Newton's law of motion subjected when a particle is subjected to certain force. And this is widely used in all branches of physics, not only in classical mechanics. And momentum space description is often suited in various fields of quantum mechanics or say for example solid state physics when a system has translational periodicity or translational invariance that is the space is homogeneous then K is a good quantum number or is a conserved quantity and that is why we resort to the momentum space or K space here K means P equal to h cross K. So, this configuration space is as I said just represented by x, y, z and the volume of this space is given by dx, dy, dz as you can see it here in this

The diagram below shows a cube, a small cube where each of the sides are dx, dy, and dz. With respect to a certain origin, there is a point at the center of the cube. It has a position defined by x, y, and z, which is not shown here, but that is what it represents. Let me try to illustrate this here. So, this point that you see here is x, y, z and so on with respect to certain origin. So, you have built up a volume around it and this volume has this, the volume is equal to the dx, dy, dz.

Similarly, in the momentum space, once again, we have this momentum given as say px, py and pz to be the center of this, this cube is has coordinates px, py, pz in this A plane defined by px, py and pz and you have constructed a volume around it and it is often written with a D tau or we can also write it with dv which is equal to d px, d py and d pz. Now, what is phase space? So, phase space is a mathematical concept. of constructing a six dimensional space which incorporate both the configuration and the momenta coordinates which means that for a single particle it will have six coordinates to go along with and these six coordinates are xyz and px py pz and now the elementary volume is a six dimensional quantity which is

dx, dy, dz, dpx, dpy, dpz, and so on. So, this is a 6 dimensional plane or space for one particle and since we consider n particles and n to be of the order of Avogadro number 10 to the power 23 or 10 to the power 24. The space is six and dimensional. So even if it looks like that, we have artificially enhanced the dimensionality in which we are going to study. But this makes a lot of things quite simpler and which is what we are going to see.

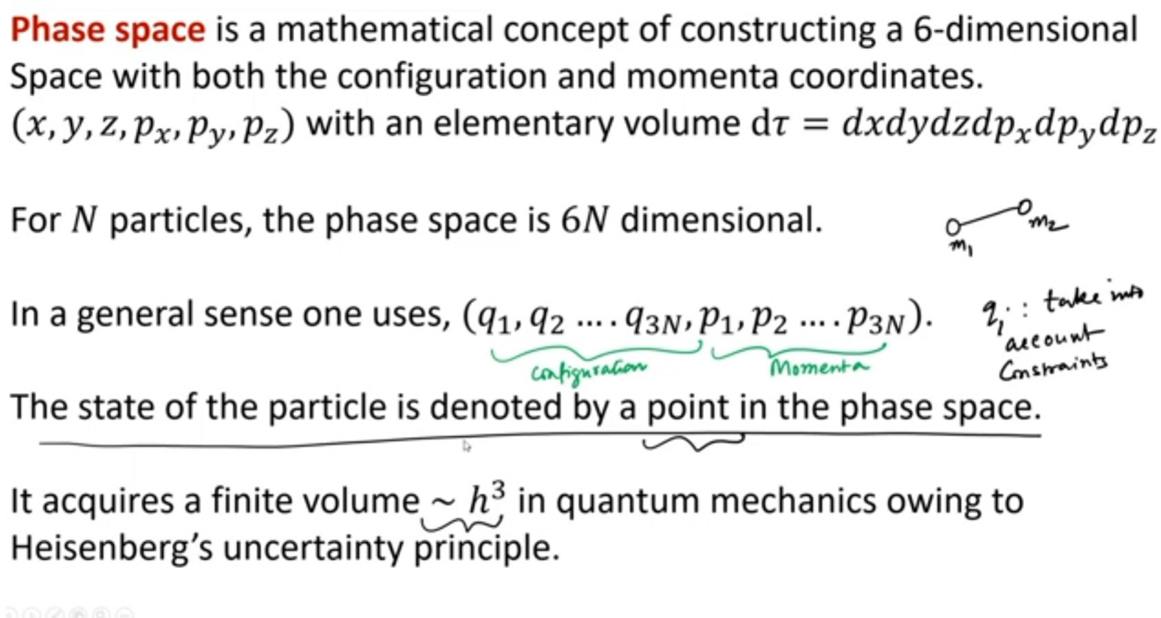
So, in a general sense, instead of using x, y, z, one uses q1, q2 up to q3N coordinates. N stands for the number of particles. As I said, there will be p1, p2, and p3N, where qs are called the configuration coordinates, and these are the momenta. And why do we shift from xyz to q1, q2? That is because these are called the generalized coordinates, and how do generalized coordinates differ from ordinary Cartesian or ordinary configuration coordinates? Because these take into account the constraints that the system possesses, okay.

So, the system may possess certain constraints. Say there is a sort of dumbbell which is in space, which means that there is a constraint that the distance between these two weights, they always remain fixed and this may actually rotate. or they may undergo translation, but with respect to one, the coordinates of one of the masses, let us call this as mass m1 and m2, the distance is always constant and there is a constraint of the problem. So, these qi's, they take into account the constraints. All right.

So, the state of the particle is very important. The state of the particle is denoted by a point in the phase space. So, the state of the particle means or the state of the system, for example, is a point in the phase space. A 6-dimensional space or 6N-dimensional space—if you put a point there, that point is your system. Maybe a classical ideal gas—that is a sort of representation of your system in the phase space. And, of course, as you know, time evolves, and the molecules of the gas would be moving around due to the kinetic energy present in them. This gas will execute a trajectory in the phase space.

So, that could be a line or that could be sort of a trajectory that we will see soon. Though it is a purely classical concept because we are talking about energy and momentum, at the same footing and which is prohibited by quantum mechanics owing to the uncertainty principle which says that if you really want to precisely determine the position of a particle then the momentum uncertainty that is a measurement of momentum yields a very huge uncertainty and this is called as uncertainty principle and delta X into delta P X will be of the order of h cross which of course we can neglect in classical mechanics, but h cross which is or h say for example, h is the Planck's constant, it cannot be ignored in quantum mechanics.

However, still if you want to have an analogy and want to sort of carry on some of the ideas of classical mechanics to quantum mechanics, then this point that we talk about in this phase space can be represented by a small volume of the order of h cube and that would sort of let you at least establish a correspondence or an analogy. So, this evolution of the particle's trajectory is given by these equations of motion. These are called the Hamilton's equations of motion. where the time evolution of the coordinates, which are called QI (the generalized coordinates), and the generalized momenta here, which are PI, are given by del H del PI and minus del H del QI, where H denotes the Hamiltonian of the system. So, if you solve them, they give you how Qi and Pi evolve in this phase space.



So, a surface in the phase space is defined by the locus of all the phase points that satisfy this relation that H of Qp, which is the Hamiltonian, which is a function of this generalized coordinate and the generalized momenta that would give you the energy which is a constant. So, is the energy of the system. So, that is the surface in a phase space and this surface either can be a hyper you know volume or it can be it is often called as a hyper cube or hyper surface or hyper volume. and so on.

So, this is a generalization of this volume from say three dimension that we are aware of to larger, much larger dimension. Okay. Often we find that it is much better not to fix a value of energy to be taking a single value. That is, you relax the condition that the energy is strictly a constant value E, but you allow a small variation of energy E. of the system and so say the system can have energy between some E minus delta to E plus delta where delta is a has a dimension of energy and is a small quantity as compared to E okay and so the trajectory of the system will be restricted in a hyperspace which is defined by these two limits okay.

Let me now sort of show you the phase space. How does it look like for a couple of simple examples? And say the first example is a mass M is confined to move in one dimension, okay. So, and it is a free mass or free particle, okay.

Further, the evolution of the particle's trajectory is governed by the Hamilton's equation of motion.

$$\dot{q}_i = \frac{\partial H\,(q_i, p_i)}{\partial p_i}$$

$$\dot{p}_i = -\frac{\partial H\,(q_i, p_i)}{\partial q_i}$$

H : Hamiltonian of the system.

A surface in the phase space is defined by the locus of all the phase Points satisfying the relation,

$$H(q,p) = E = \text{constant}$$

Where E denotes the energy of the system.

So, you can add this thing, it is a or we will just add it here, it is a free particle and the moment I see it is a free particle, it means that the energy is given by E equal to P square over 2m because it is free the only energy that it has the kinetic energy and P is the momentum and m is the mass as it is been say. So, this tells you that if you want to know the phase space of this particle which is confined to move in 1D free particle. So, this P becomes equal to a plus minus root over of 2 mE and that gives you that there are these two energy values. So, this is your, now we can call it X or Q, whatever you want to call it.

If instead of a fixed energy, we consider a small variation of energy of The system, namely,

$$E - \Delta \leq E \leq E + \Delta$$

Then the trajectory of the system will be restricted in a hyperspace defined by these two limits.

And so, this is a plus root over 2 m E, and this is minus root over 2 m E, and this is the p-axis. So, it is a p-q plane, and we are just talking about one particle. So, this is the phase space of this particle. So, they are restricted between two values of p which are plus root over 2 m e and minus root over 2 m e. And just like as we have said, if you give a little bit of energy variation so that they are really allowed to be confined in this region and similarly in this region, then this is of course, of the width

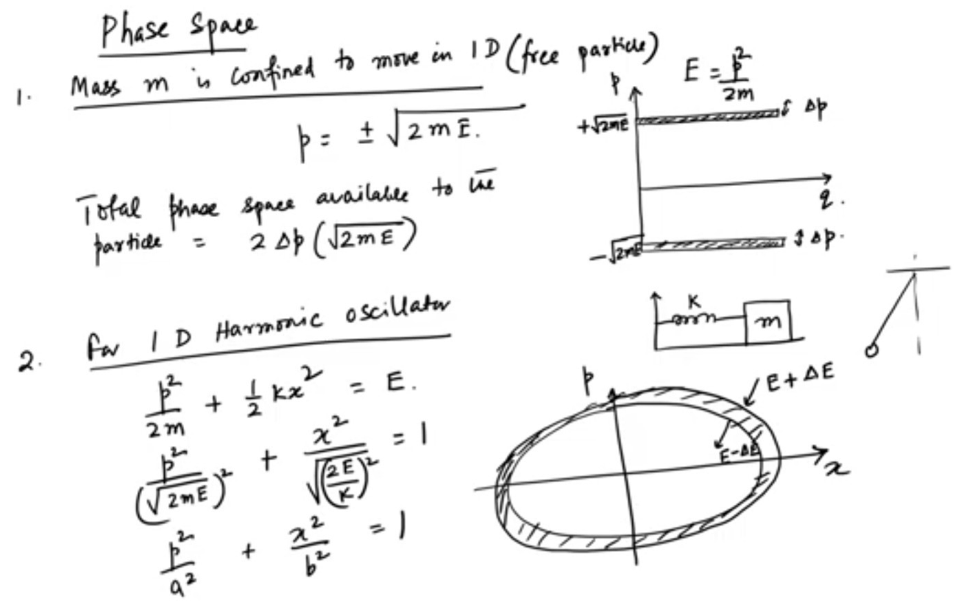
this is a delta p, and this is delta p as well. And so, the total phase space is for this particle —there is just one particle, as I said, and that too in one dimension. So, things are extremely simple. So, the total phase space available to the particle is equal to 2 into delta p

into root over 2 m E. The 2 you understand because there are 2 of them at plus root over 2 Me and minus root over 2 m E, and delta P is the width. So, that shaded area is the phase space that is available to the particle to move in. Second, the more familiar example that is there everywhere. So, for a 1D harmonic oscillator,

So what I mean by 1D harmonic oscillator, it could be a mass spring system say for example like this. So there is a rigid wall which has a spring attached to it and there is a mass that is attached to it and this is offspring constant K or it could be a pendulum say which is made to you know oscillate in this vertical plane. So, the energy of that is given by the P square over 2m, but now it is not only P square over 2m, there is a half kx square energy which is associated with the spring. Let us just talk about the spring-mass system. This is equal to the total energy, okay. So, if energy is constant, then of course, you have this: it varies with P and X as P squared over 2m plus half kx squared.

Now, what I do is that I will do like this root over 2 m e whole square plus x square by root over 2 e over k square that is equal to 1. I will write it in this particular fashion, and this is nothing but the equation of an ellipse and this has in the PX plane remember that we are writing it X back to the original notation for the configuration coordinates one could write it as Q as well just to loosely writing it as half KX square so this is the P axis and this is the X axis or Q axis it will be a ellipse which has a semi-major axis as root over 2 m e square. So, this is like P squared over A squared plus X squared over B squared equals 1.

So, you have a semi-major axis and a semi-minor axis there. And again, if E is made to, you know, sort of vary between some E plus delta to E minus delta, we can write it as— so this is the available phase space for the particle. So, this is the phase space available is between these two ellipse which this is E plus delta E and say this is E minus delta E or just E that would be also be fine. But we just write it in a symmetric fashion. So, it is between E plus delta E and E minus delta E. So, these are the concepts of phase space that you often get.



Let us just look at the second thing that we have talked about that is this microstates and macrostates as you see at the bottom of this slide and let us try to explain what are these macrostates and microstates. The state of a system is completely specified by the macrostates. which means that it could be the pressure, volume and temperature of a system or the energy, volume and number of particles of the system and so on. So, they sort of tell you that this gas has a classical ideal gas has a certain pressure, volume and temperature or certain energy coming from the momentum. So, make sure that this capital P is used for pressure throughout our discussion and small p is momentum.

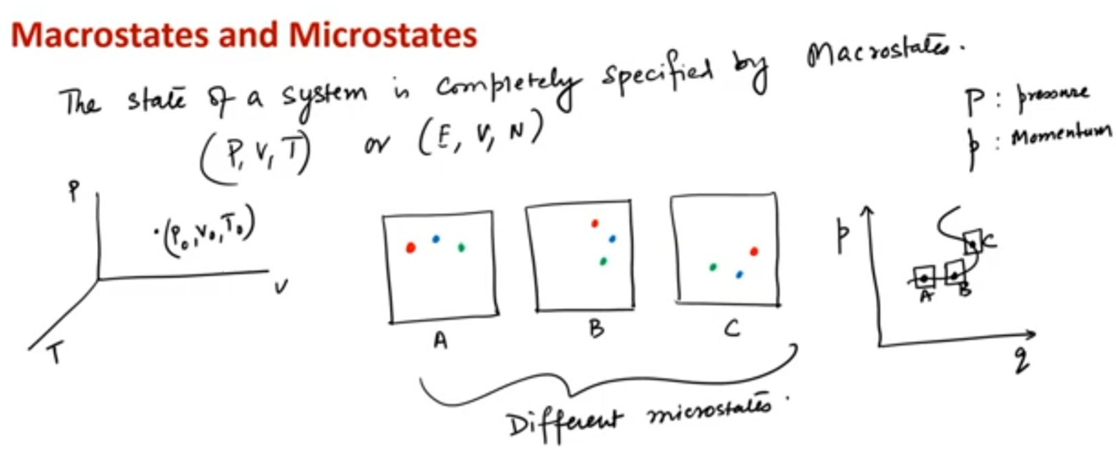
So, please make this distinctions in your when you read it or when you work out things. Now, this state of the system described by this PVT or EVN, they say nothing about the internal structure of the gas, it just tells you about the state of the gas. And if you sort of if I have to give some examples, so let us say that we have a PV and T. And there is a certain point which corresponds to P0, V0 and T0 of a gas. Now, these are the macroscopic parameters that specify the state of the gas that you have made a measurement and you have got a value which is P0, V0 and T0.

Okay. But this particular macrostate may correspond to very large number of microstates that is suppose we have we talk about a gas like this. We will just draw a few boxes here and only look at say for example, a few particles a and this is one particle marked by red and there is one particle marked by blue and there is one particle marked by green. There are, of course, Avogadro number of particles.

We cannot draw all of them, but we simply draw three particles. And in this diagram, the schematic diagram that you see, it represents the same gas with P0, V0, and T0. However, these particles, which we have marked in red, blue, and green, occupy different configurational positions, or you can say positions in the phase space. We are just showing them inside a box. So, it might give you the feeling that we are only talking about the configuration space, but that may not be true.

It is, we may be talking about the So, in the phase space, these three descriptions of the gas are distinct. So, they correspond to different parts or different points in the phase space. So, let me draw that phase space as well and so there is a P and sorry this is momentum. So, we will call it P, and now we go back to our original generalized coordinates.

So on. So, this may be the trajectory of the particle and this is your A, let us call it as A and this is B and this is C. So, this could be B and this could be C. So, A, B and C, this correspond to different points in the phase space. So, these are, this is the same gas as we have in A, B and C, but their internal structures are different and these corresponds to different microstates. Okay. So, and every point on the phase space trajectory will give you a different microstate.



Okay. And so, a macrostate in general is comprises of very large number of, a macrostate comprises of a very large number of microstates. Okay. Let me give you another example. So, let us have a spin configuration, or simply you can talk about magnetic moment.

Let me just go back and just reflect one more time on this the same slide that we have been on. I mean, you might wonder that we have, of course, colored some molecules of the gas by red, blue, and green. Is it really possible? I mean, is it sort of, can we do that? Are we allowed to do that?

And the answer is that, yes, in classical physics, all these particles are known to be distinguishable. We can label them as per our wish. But however, as soon as you go to quantum mechanics or quantum physics, the particles become indistinguishable. And indistinguishable particles cannot simply be marked by red, blue, and green. We will have to, you know, follow that procedure of indistinguishability and we will do that when we come to quantum statistical physics.

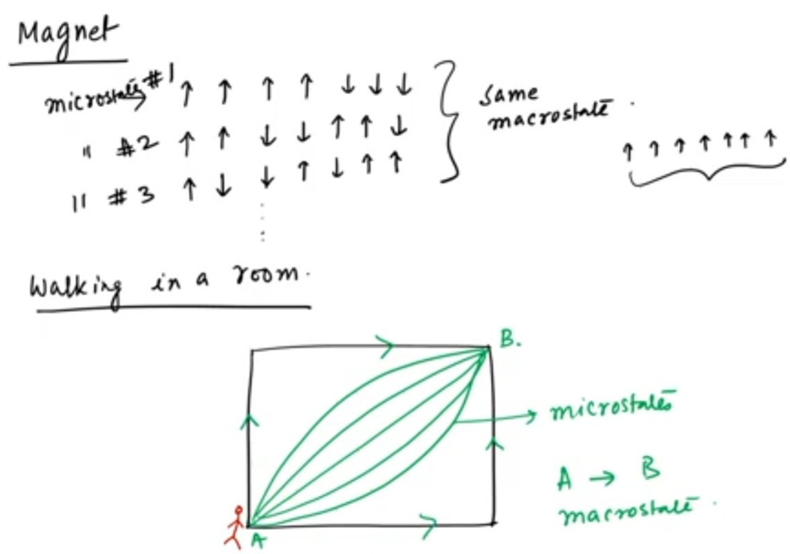
Okay, coming back to the second example that we saw, let us talk about a magnet. And there are a number of spins, and let me sort this out—so there are four magnetic moments or spins, if you like. They are pointing up, and three are pointing down. So, I can have this, and this is another configuration of the same thing, and this is another configuration of the same thing. And there are many configurations that one can find or one can write down.

So, the same macro state with, you know, the net magnetic moment to be say one unit because there are four up and three down. So, there is eventually one magnetic moment upward. or pointing upward and so they correspond to all of these configurations, they correspond to the same macrostate. But however, each one of them is a distinct microstate. So, this is one microstate, number 1, and this is microstate number 2.

and this is microstate number 3 and so on and we can put you know a large number of combinations with here and each will give rise to a distinct microstates where the first spin to the you know the seventh spin are ordered either up or down to give you the same magnetic net magnetic moment which is one unit pointing upward okay. So, let me give you another example of say walking in a room. Imagine yourself that you are standing in a square room or rectangular room, it does not matter and you are right here. And you are asked to go from point A to a point B. OK.

And, you know, so the macro state would correspond to these two extreme positions that one has to go from A to B. But then you see that there are so many micro states present. You can you can go from this side to this and then this to this. You can go like this. You can go like this. You can go like this and you can go like this.

this and you can go like this and you can go like a large number of ways. So, the number of ways that you can go or rather walk in order to reach from the point A to point B, they denote the microstates. So, these are the microstates of the system and the macrostates are A to B is a macrostate. I think it is by now clear that each macrostate, which is an overall course description of the system, that corresponds to a large number of microstates. And these microstates are very important because these microstates will eventually be related to the entropy system.



of the system, as we will see, you take the log of the number of microstates and multiplied by the Boltzmann constant, you get entropy of the system. So, that tells you that a ferromagnet, which is represented by only one configuration where all the spins are pointing up, I mean what I mean by ferromagnet is that all the magnetic moments are pointing in the same direction. This has, there is just one way that it can be done and so this has a number of microstate is equal to 1 and the number of microstates equal to 1 and when you take a log of 1, you get a 0. So, the entropy of the system is 0.

And by now, we know that the entropy is related to the disorder present in the system. So, this system is least disordered and we know that it is an ordered system. An ordered system, completely ordered system is not a disorder system and that is why the entropy is equal to 0. So, I will stop here and thank you. Amen.