Computational Physics

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Lecture - 16
Monte Carlo Simulation Introduction Part 01

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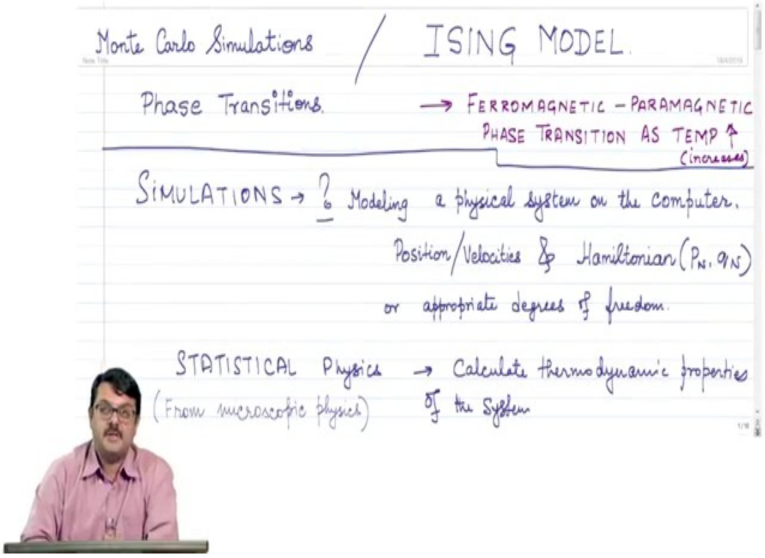

Monte Carlo Simulations / ISING MODEL.

Phase Transitions. → FERROMAGNETIC – PARAMAGNETIC PHASE TRANSITION AS TEMP ↑ (increases)

SIMULATIONS → i.e. Modeling a physical system on the computer.
Position/Velocities & Hamiltonian (p_N, q_N)
or appropriate degrees of freedom.

STATISTICAL Physics → Calculate thermodynamic properties of the System
(From microscopic physics)

So, hello everybody and welcome to the third module of this course where we shall be learning about Monte Carlo simulations. And in particular, we shall model the Ising model, use the Ising model for our Monte Carlo simulations. Now, what is the Ising model? It is basically a model Hamiltonian to understand Ferromagnetic to Paramagnetic phase transitions as one increases the temperature.

Using these Monte Carlo simulations by which we should model the Ising model, we shall be aiming to understand the phenomena of phase transitions. So, the Ising model shows Ferromagnetic to Paramagnetic phase transitions and the broad idea is that if you understand the phase transitions in the Ising model, one can extrapolate similar ideas. So, we can learn the language of phase transitions and extrapolate these ideas to understand more complicated phase transitions behavior.

Now, I understand, right at the beginning I introduced a large number of terms with which you might be unfamiliar with. So, I shall basically go through each of these terms and explain what they mean, . So, what does the word simulation mean? So, by simulation the idea is to model a physical system on the computer and as you change parameters like temperature, pressure, magnetic field, etcetera on the computer, where these things are also modeled in a program on the computer, the system basically shows behavior, change in behavior analogous to the real system and then you are basically trying to model the system on the computer and understand its behavior. For that one needs essentially the appropriate degrees of freedom.

Now, suppose you are going to model the liquid gas transition, then you basically need to define the position and velocity of end particles in a simulation box. Of course, I shall discuss all these in further detail; give the effective interaction energy or the Hamiltonian of interaction between the different particles of the box and then these particles basically interact via this Hamiltonian and they move around in space. So, they collide with each other, they change their positions, they change their velocities and then using appropriate statistical physics. So, you have specified the microscopic degrees of freedom and using the language of statistical physics, one can calculate thermodynamic properties of the system and then compare with nature or with experiments.

Now, if you are using the right Hamiltonian, you are using the right interaction, you are modeling it appropriately, your model simulations will show the appropriate behavior. And now, you have access to all the microscopic degrees of freedom from which you calculate whatever thermodynamic properties you want to calculate and basically develop an understanding of the system, all right. Now, just to remind you what does statistical physics do? It basically connects microscopic degrees of freedom or you start from the microscopic physics and it gives you a mechanism to calculate thermodynamic properties of the system which are typically measured in the lab, ok.

So, before we even discuss the Ising model which is a model Hamiltonian to understand Ferro magnetism and before we actually talk about simulations, we shall basically revise or since you might be coming all coming from different backgrounds with different statistical physics one course, we shall discuss what is phase transitions, give you some appropriate background about the physics of phase transitions. And only after that background we shall discuss or write down the Ising Hamiltonian, discuss the physics of it, discuss Ferromagnetic to Paramagnetic transitions and then we shall get down to the calculation or the simulation details how are we going to model this, model Hamiltonian on the computer to understand Ferromagnetic to Paramagnetic phase transitions. So, that is the plan. So, the first half an hour or more is going to be discussing phase transitions, statistical physics and so on so forth.

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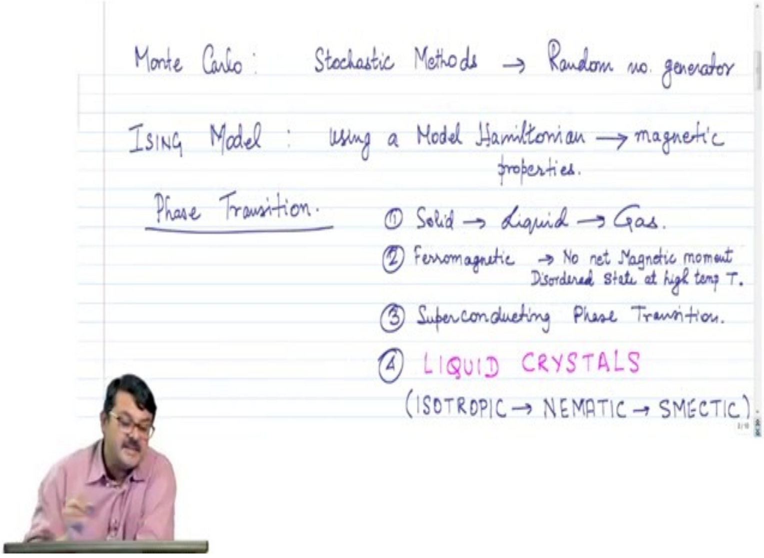

Monte Carlo : Stochastic Methods → Random no. generator

ISING Model : using a Model Hamiltonian → magnetic properties.

Phase Transition.

① Solid → Liquid → Gas.

② Ferromagnetic → No net Magnetic moment Disordered state at high temp T.

③ Superconducting Phase Transition.

④ LIQUID CRYSTALS (ISOTROPIC → NEMATIC → SMECTIC).

Before I discuss phase transitions, let me tell you what do I mean by Monte Carlo simulations. Now, even in the first or the second module you have you know that Monte Carlo method is essentially solving a problem using stochastic method. So, basically there will be a random number generator. So, even in our simulations and Monte Carlo simulations, we shall use a random number generator to access different microstates of the system. So, when we model a Ferro magnet we shall basically make our model system access different microstates, and how these microstates will be accessed it will be a stochastic method using a random number generator.

I already told you that Ising model is a model Hamiltonian which basically shows or mimics the magnetic properties of using the Ising model we can understand, the Ferromagnetic phase transition Ferromagnetic to Paramagnetic state as you increase the temperature of the system and this is a good method to understand phase transitions. But let us first discuss what do I mean by phase transition, what is its basic behavior, what do you understand by phase transitions.

Now, you might have already have and have had an intuitive idea with the meaning of the word phase. So, you know that basically when you have ice, it is in a solid phase and when you increase the temperature it becomes water or it becomes goes to the liquid phase and when you increase the temperature to at even higher temperatures above 100 degree centigrade, it becomes the gas phase. So, these are various states of matter. They have different properties. Microscopically they have different symmetries, and when you change an external field in this case the temperature basically the system goes from one phase to the other phase to the other phase.

You might have also known or heard about the Ferromagnetic phase transition. So, you have all played with a bar magnet and at room temperatures it shows a finite magnetic moment. If you take a bar magnet it likes to point along the north if you suspend a bar magnet using a thread, it will it basically likes to point along the north pole or rather the not the north pole, but the basically magnetic north pole and you know that if you increase the temperature beyond a certain critical temperature, the magnetic moment the magnetized state of that iron is lost. So, basically again when you increase the temperature, there is a phase transition from the Ferromagnetic state to a high temperature state where there is no net magnetic moment. Microscopically the spins or the magnetic moments point in all possible directions at high temperature and how and why that happens is what we shall be exploring through our Ising model simulations.

You might have also heard about the superconducting phase transition. There are some materials like mercury which at high temperature are conducting, but when you cool down the system below a certain critical temperature the resistivity essentially goes to 0, the conductivity becomes infinite and you say that it has changed from a normal metal to a superconducting phase.

So, these are things which you might have a already heard about let me introduce to you some phase transitions in some liquid crystals. These liquid crystals are the same liquid crystals that you might know about from liquid crystal displays liquid crystal lcd tvs and they are basically the arrangement of the molecules, and I shall discuss this in greater detail goes from the isotropic to the nematic to the smectic phase. What are they?

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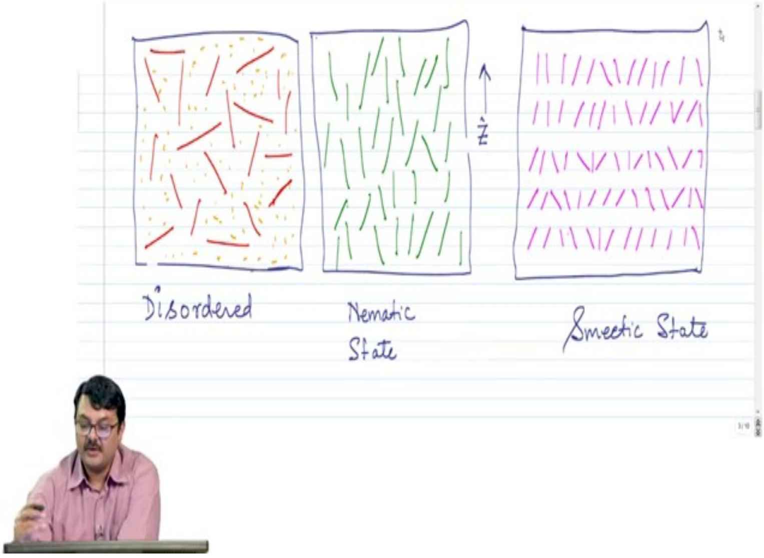

So, what are these things? What are liquid crystals? And what are these phases? What am I talking about? So, basically the idea of liquid crystals the constituent, so the constituent of liquid crystals are essentially made up of long rod like molecules like these, . And these are typically dispersed in a background fluid, these orange dots essentially then denote a background fluid and these rod like molecules undergo Brownian motion in the fluid and they are point pointed in all possible directions.

Now, as they undergo Brownian motion they are not only change their position from say here to here, but even the axis, so you see if there is a rod like molecule you can define an axis along the rod. And these axis along the rod also undergo Brownian motion and basically the axis can point in all possible directions and this is because of the bombardment of the background fluid, and then you say that it is in the so called disordered state.

Now, if you increase the density of these rod like molecules in the system, what happens is these rod like molecules tend to orient themselves along a particular direction say that Z direction, ok. So, in this state which is called the nematic state or the nematic phase what you have is the average orientation of the axis is along the Z direction, but the position can change. So, the position is doing a Brownian motion. So, it can move from any one point in space to the other. The axis can also change this that is also doing some

Brownian motion of course; there is some rotational Brownian motion. But on an average you see in this picture that the axis is all pointing along one particular direction.

So, you see that that there is change in symmetry from the so called disordered phase to the nematic phase where there is ….. So, in this nematic state there is no positional order, yes, the there can be in any point in the liquid just like a liquid, but you have got orientational order. So, there has been a change of phase and there is been change in microscopic symmetry, there has been a change in order the microscopically in the system.

Now, if you increase the density of these molecules even further and assuming that the molecules are all of the same size, they can go in the so called smectic state. In the smectic state they basically not only point on an average along a particular direction say the Z direction, but they also align themselves up in layers. So, this is one layer, this is one layer, this is one layer. So, in a layer the particles can move around within that layer freely like a liquid. There is an average orientation axis of course, there are fluctuations, but there is an average orientation axis.

So, in the x and y direction, assuming this is x and this is y, it is moving around in a liquid, but there have some order which has been picked up along the Z direction, ok. So, if you look at the density, you will see a density of these molecules, there is some density modulation from here to here to here to here. So, there is increase in model in the density here and lesser density of these molecules in between these layers.

So, again previously you had examples where you had phase transitions when the temperature was changed the solid liquid gas or the Ferromagnetic or the superconducting, but here you see that when you increase the density of these rod like molecules you are going from the so called disordered phase to the nematic phase to the smectic phase, ok.

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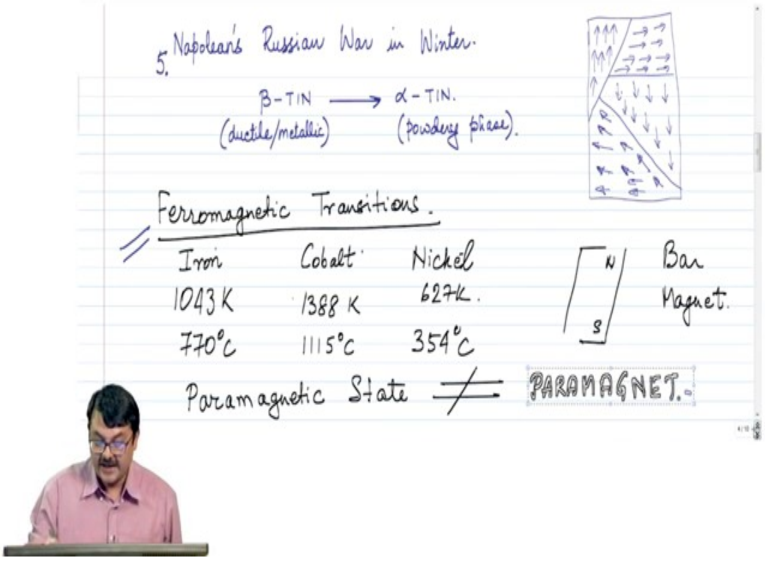

5. Napolean's Russian War in Winter.

β-TIN $\longrightarrow$ α-TIN.
(ductile/metallic) (powdery phase).

Ferromagnetic Transitions.

Iron	Cobalt	Nickel
1043 K	1388 K	627K.
770°C	1115°C	354°C

Paramagnetic State $\neq$ PARAMAGNET.

So, while it is interesting enough to understand from a basic point of view basic physics point of view why these phase transitions or how these phase transitions happen. It is important to understand phase transitions also for industrial purposes and here just for the fun of it, I give you an example where lack of understanding of phase transitions led to defeat in a war. So, Napoleon when he basically attacked Russia 200 years ago, and he decided to attack Russia in the winter basically the soldiers were varying some coats.

So, this coat had buttons which was made up of tin, ok. And when he reached Russia to fight his war Russia's far colder than the other parts of Europe basically these buttons which were in the so called beta tin phase and which is a ductile and metallic and behaves like a normal metal that underwent phase transition at lower temperatures into so called the alpha tin and that is his powdery face.

So, basically the powder the buttons become powders and fell off, and that was not very comfortable for of course, the soldiers to fight in that freezing cold. Of course, I am not saying that that was the only reason he lost the war. The point I am trying to make is that understanding phase transitions also has implications and ramifications in the real world. So, you need to understand the properties of materials, ok.

With that background with this basically idea examples of these phase transitions, let us focus on Ferromagnetic phase transitions and let us discuss about phase transitions in greater detail, where we shall basically discuss the phase Ferromagnetic phase transition.

Now, you already know and you have all played with a bar magnet in all probability where basically one has the so called north pole and then there is the south pole, and you bring two bar magnets together north pole to north poles repel each other and you know that the bar magnet is magnetized, ok.

Of course, you have also iron which does not show any magnetic properties and that is because basically a bar magnet has domains, so room temperature iron, at room temperature is always magnetized. But you can also have iron where you have different domains different regions within the bar magnet where the magnetic moments are pointing along different directions like this or like this or like this on like this in different directions so that on an average you are seeing no magnet a net magnetic moment.

But when you pass a DC field or suppose you stroke a bar magnet with another magnet then the magnetic moments and these different domains essentially start pointing along the same direction. So, as a result you see a magnetized iron. But if you heat iron above 770 degree centigrade which is 1043 Kelvin you see you will see that the iron rod a magnetized or iron rod loses its magnetic properties, it does not show any net magnetic moment. And the question is how and why, what is happening within the iron that you are that the iron is unable to show its magnetic property.

Similarly, if you have cobalt and if you heat it above 1115 degree centigrade, then again it is Ferromagnetic at room temperatures, but above this temperature it loses it is magnetic properties, right. It does not remain a Ferro magnet anymore. And nickel is also a Ferro magnet and it loses its magnetism above 354 degree Kelvin. And we say that above these so called critical temperatures of 770, 1115 or 354 the iron or the cobalt or the nickel reaches a Paramagnetic state.

Now, I want to clarify and I want to emphasize that a Paramagnetic state is not the same as a para magnet. So, in a para magnet there is no effective interaction between the spins and it does not show any net magnetic moment at any temperature unless you switch on an external magnetic field. So, in what happens in this case in a paramagnet, due to thermal fluctuations basically all the magnetic moments in a paramagnet point in different directions and as a result you see no net magnetic moment, these spins are not interacting with each other or the magnetic moments are not interacting with each other.

For a Ferro magnet the interaction, there is an interaction between adjacent spins, ok, so that interaction always remains. But above a certain critical temperature given in these 3 cases what happens is that the thermal fluctuations dominates over the Ferromagnetic interactions we shall discuss this in greater detail, and it reached and it behaves like a para magnet which means that there is no net magnetic moment between the spins.

Even though there is interaction between the spins or the magnetic moments in a Ferromagnetic, which tries to align the spins in the same direction. So, basically what I want to say, that in a Ferromagnetic case when you reach when you increase the temperature below a certain critical temperature, it loses its effective magnetic moment and it reaches the Paramagnetic state and that is not the same as a Paramagnetic material. I just wanted to emphasize this. So, the high temperature disordered state is called the Paramagnetic state.

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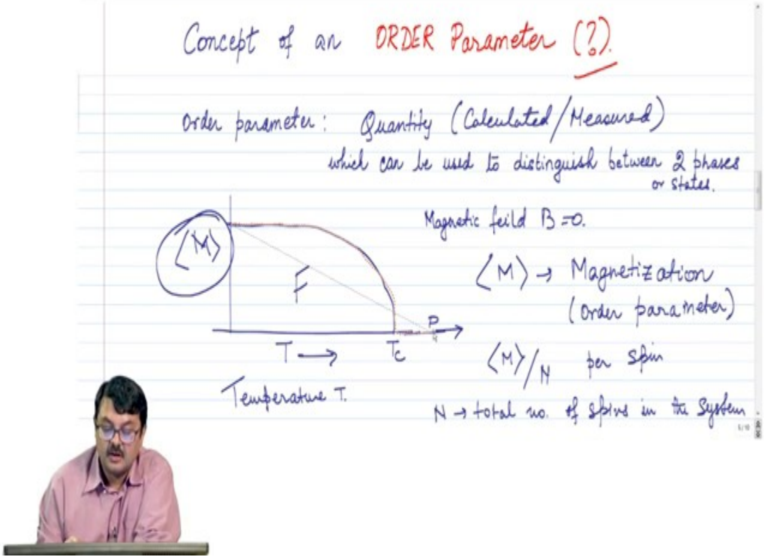

Concept of an ORDER Parameter (?)

Order parameter: Quantity (Calculated/Measured) which can be used to distinguish between 2 phases or states.

Magnetic feild $B = 0$.

$\langle M \rangle \rightarrow$ Magnetization (order parameter)

$\langle M \rangle / N$ per spin

$N \rightarrow$ total no. of spins in the System.

After this before we go on discussing phase transitions in greater detail I need to introduce the idea of an order parameter, ok. So, what is an order parameter? It is a quantity which can be calculated or measured in experiments and this quantity can be used to distinguish between the two states or the two phases. So, basically it is a quantity which will be 0 in one of the phases and will have a finite value in the other phase.

So, when we are discussing Ferro magnetism, magnetization can be used the quantity magnetization, the effective magnetic moment of the system can be used as an order parameter at low temperatures the magnetization, the average magnetization shows a finite value at 0 temperature. So, basically what is plotted on the y axis you are plotting the magnetization which you can define as the order parameter to characterize a Ferromagnetic to Paramagnetic transition.

So, on the y axis there is magnetization, on the x axis there is temperature and at 0 temperature basically all the magnetic moments in a Ferro magnet will be pointing in the same direction the magnetic moment will be the maximum. But as you increase the temperature you will see that the magnetic moment slowly decreases and above a certain temperature is called the so called critical temperature T c and the magnetic moment will go to 0, right.

For calculation purposes, so that is what you would measure in the, so this is what you would measure in experiments. For calculation purposes one can also use the magnetic moment per spin, N being the number of total number of spins in the system as the order parameter and we can calculate what is the average magnetic moment per spin and that will show some finite value at low temperatures and above the critical temperature its value will go to 0. There are certain advantages in using this quantity. We shall discuss it as we shall go along, ok.

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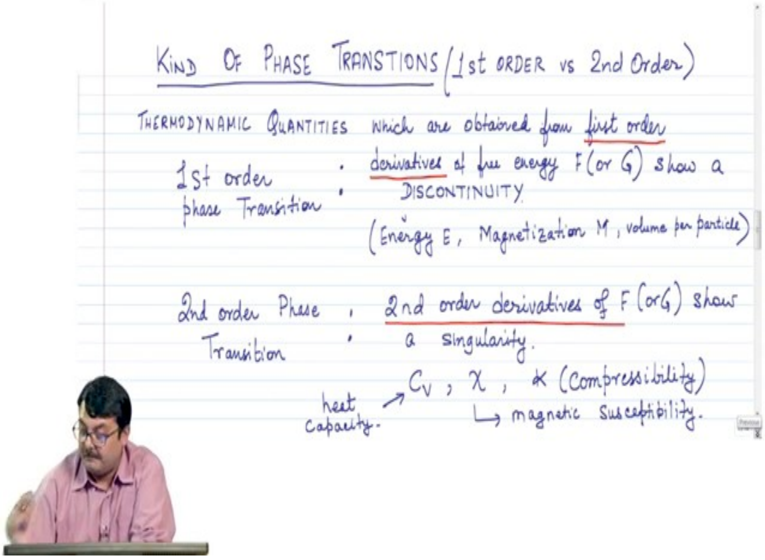

KIND OF PHASE TRANSTIONS (1st ORDER vs 2nd Order)

THERMODYNAMIC QUANTITIES which are obtained from first order

1st order phase Transition : derivatives of free energy F (or G) show a DISCONTINUITY

(Energy E, Magnetization M, volume per particle)

2nd order Phase Transition : 2nd order derivatives of F (or G) show a singularity.

heat capacity → C_V , χ , κ (Compressibility)

↳ magnetic susceptibility.

So, basically we would say that the magnetic moment here is finite and goes to 0 above the temperature and it is an order parameter. And next, what I shall introduce the idea of is kind of phase transitions. You have the so called the first order phase transitions and you have this so called second order phase transitions.

I shall discuss that basically the Ferromagnetic to Paramagnet take transition at T c is a second order phase transition. But, what are first order phase transition and what is a second order phase transition? So, in a first order phase transition thermodynamic quantities which are obtained from the first order derivatives of the free energy they show a discontinuity. What do I mean by that? What are the first order derivatives of the free energy?

Quantities like the average energy, the internal energy of the system, the magnetization, if you are talking about a Ferromagnetic sample magnetization. If you are talking about a liquid gas phase transition then volume per particle, these quantities the average about the thermodynamic averages can be obtained by taking first order derivatives of the free energy or the Gibbs free energy depending upon what ensemble you are working on. Why is that we shall discuss it.

And what are say a second order phase transition? Quantity is like the heat capacity, the magnetic susceptibility or the compressibility which are second order derivatives of the free energy or the Gibbs free energy. So, F being the Helmholtz free energy and G being the Gibbs free energy these quantities like C v chi and compressibility are essentially second order derivatives of the free energy and they show a singularity, ok. For second order phase transitions the quantities is like energy magnetization these do not, I mean whatever be the relevant thermodynamic quantities they do not show any discontinuity. Why did I say energy magnetization, these are first order derivatives of free energy?

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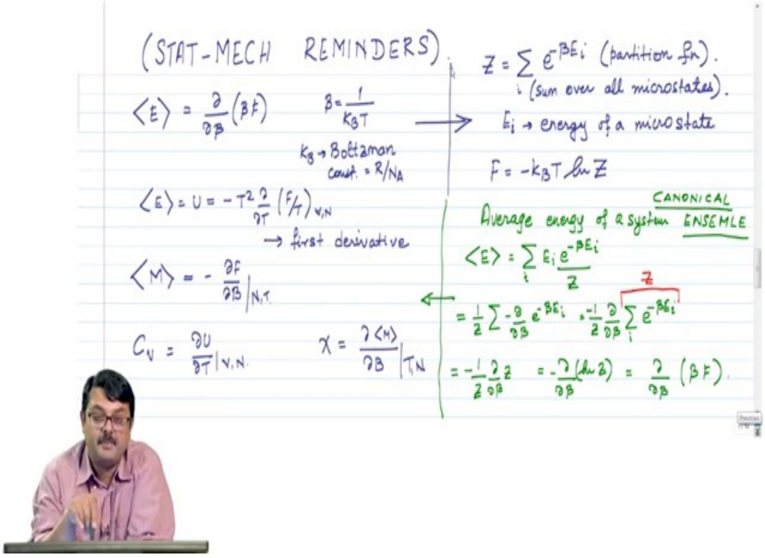

(STAT-MECH REMINDERS)

$\langle E \rangle = \frac{\partial}{\partial \beta}(\beta F)$ $\quad \beta = \frac{1}{K_B T}$

$K_B \rightarrow$ Boltzman const. $= R/N_A$

$\langle E \rangle = U = -T^2 \frac{\partial}{\partial T}(F/T)_{V,N}$

→ first derivative

$\langle M \rangle = -\frac{\partial F}{\partial B}\Big|_{N,T}$

$C_V = \frac{\partial U}{\partial T}\Big|_{V,N}$ $\quad \chi = \frac{\partial \langle M \rangle}{\partial B}\Big|_{T,N}$

$Z = \sum_i e^{-\beta E_i}$ (partition fn). (sum over all microstates).

$E_i \rightarrow$ energy of a microstate

$F = -k_B T \ln Z$

Average energy of a system CANONICAL ENSEMLE

$$\langle E \rangle = \sum_i E_i \frac{e^{-\beta E_i}}{Z}$$

$$= \frac{1}{Z}\sum -\frac{\partial}{\partial \beta} e^{-\beta E_i} = -\frac{1}{Z}\frac{\partial}{\partial \beta}\overbrace{\sum_i e^{-\beta E_i}}^{Z}$$

$$= -\frac{1}{Z}\frac{\partial}{\partial \beta} Z = -\frac{\partial}{\partial \beta}(\ln Z) = \frac{\partial}{\partial \beta}(\beta F).$$

Let me just quickly remind you. There is a quick recap. So, it is even title Stat-Mech reminders. Let me remind you that when we are discussing a system which is basically in the canonical ensemble, the average energy of the system can be defined as del del beta of beta times the free energy. What is beta? It is 1 by K B T, ok.

So, how do you obtain that? I shall just remind you that Z is the partition function. Statistically, you must have at least come across the partition function in your stat phase is one course. Z is the partition function and is defined as the sum e to the power minus beta E i, sum over i where the sum is over all microstates that the system can access and E i is the energy of each microstate.

Now, if you can calculate the partition function and in some cases in the simplest cases you can and in more complicated cases you cannot, and that is why you do simulations. But in principle if you manage to calculate the partition function then you can write down the free energy F, the Helmholtz free energy F as minus K B T of log of Z, log of the partition function. And if you can write down explicitly, if you can calculate the free energy then by taking suitable derivatives with respect to beta, beta being again the 1 by K B T, K B being the Boltzmann constant then you can calculate the average energy of the system.

Why are you able to calculate that or how are you able to calculate that? I shall just remind you that the average energy of the system can be written in by this expression. It is basically a sum over all microstates, energy of the microstates and this is the probability of accessing e to the power minus beta E i by Z is the probability of accessing that microstate, right. This is the general formula.

So, different microstates are being access with different probabilities depending on the energy of the system and you do a weighted average of the energy of each microstates and that is how you get the average energy. And that can be written this expression can be written as 1 by Z del del beta when you take a derivative with respect to beta, beta being as I told you 1 by K B T. When you take a derivative with respect to beta, you basically get this energy comes out and I have put in a minus sign to keep track of the right signal the signs. This can be written like this.

And the new since you are taking a derivative with respect to beta, you can pull it out of the summation sign, the summation is over all microstates and if you can write that you shall see that summation over i e to the power minus beta E i is nothing but the partition function which we wrote down here, right. So, immediately you can write this as 1 by Z del del beta of the partition function. 1 by Z del Z del beta can be written as del del beta of log Z with a minus sign and log Z lon Z is nothing but beta times F. I am using this expression. I am just using log Z and just basically writing minus k beta which takes care of the minus sign.

So, what I what I have shown here is you should have done already in a Stat-Mech course that the average energy of the system can be written as del del beta of beta into free energy. If you write beta, if you use this relation you can also write this average energy of the system in terms of T square T being the temperature del del T of F by T. I have done nothing, but taken the converted this derivative, converted this derivative with respect to beta to with respect to temperature. Using very similar methods please check it up, look up your Stat-Mech book. The magnetization can be written as del F del B, B being the magnetic field, ok. So, if you have a magnetic system you take the first derivative with respect to B. Using statistical physics one can show that the average magnetization can be written.

You see that both average energy, magnetization, these are essentially the first derivatives of the free energy. And what I had said that first order transitions are those where the first order derivatives of the free energy show a discontinuity.

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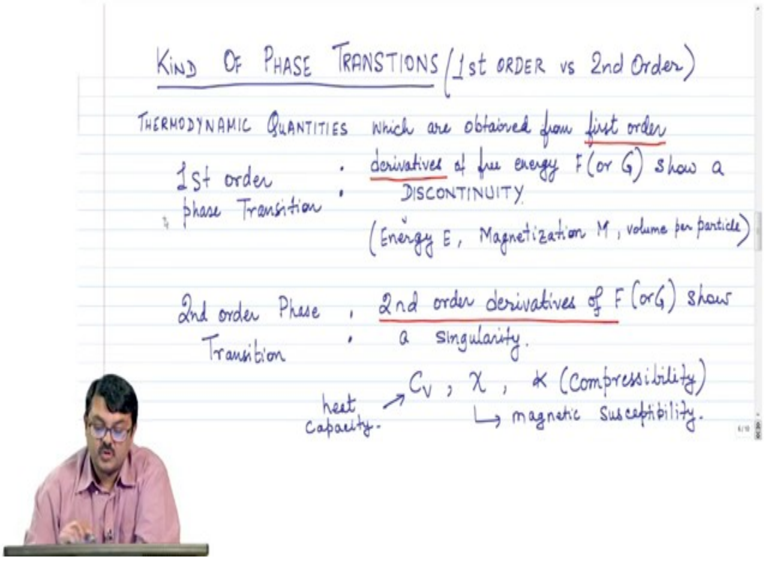

KIND OF PHASE TRANSTIONS (1st ORDER vs 2nd Order)

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2nd order Phase Transition : 2nd order derivatives of F (or G) show a singularity.

heat capacity $\nearrow C_V$, χ, κ (Compressibility)

$\hookrightarrow$ magnetic susceptibility.

Now, in a Ferromagnetic to Paramagnetic transition, the first order derivatives of the free energy the average energy and M they do not show a discontinuity. What is seen is it changes continuously, but C v which is the second ordered derivative. So, what is C v? It is basic del U del T, del U is the, U is the internal energy which is basically a measure of the average energy of the system. So, C v or chi, chi is the basically magnetic susceptibility, del M del beta, right. So, these show a singularity, ok. So, the magnetic the Ferromagnetic to Paramagnetic transition is a second order phase transition because the first order derivatives do not show any jump. If they show a jump as when water changes to gas when you increase the temperature it is associated with a latent heat, ok.

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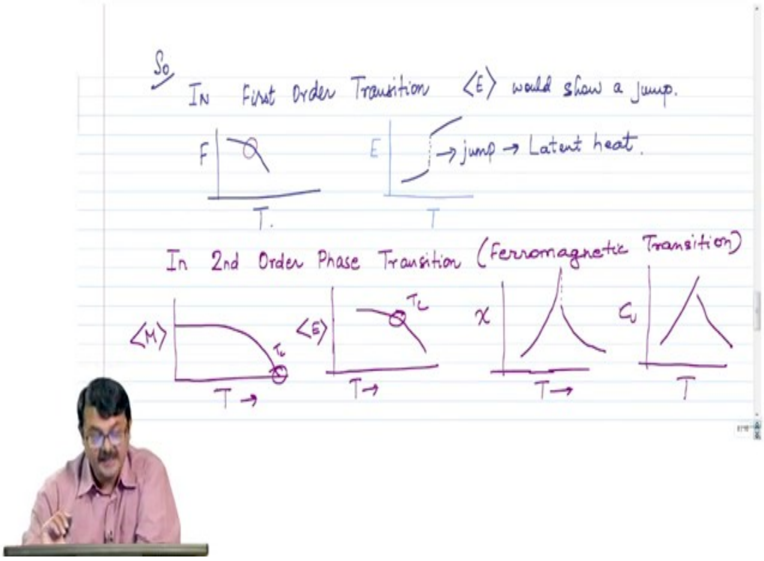

So, In First Order Transition $\langle E \rangle$ would show a jump.

→ jump → Latent heat.

In 2nd Order Phase Transition (Ferromagnetic Transition)

There is a jump in the first order derivatives, it is associated with the latent heat, but a Ferromagnetic to Paramagnetic transition is essentially a second order phase transition.