Foundations of Computational Materials Modelling
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Lecture 21
Basic Introduction to Mechanics

Good afternoon. Let us continue from where we left of. So, yesterday, we introduced a little bit of statistical mechanics and told you that this omega, number of ways a particular microstate can be reached is essentially an important quantity and with that you can basically derive the thermodynamics of a system and we showed that for a ideal gas.

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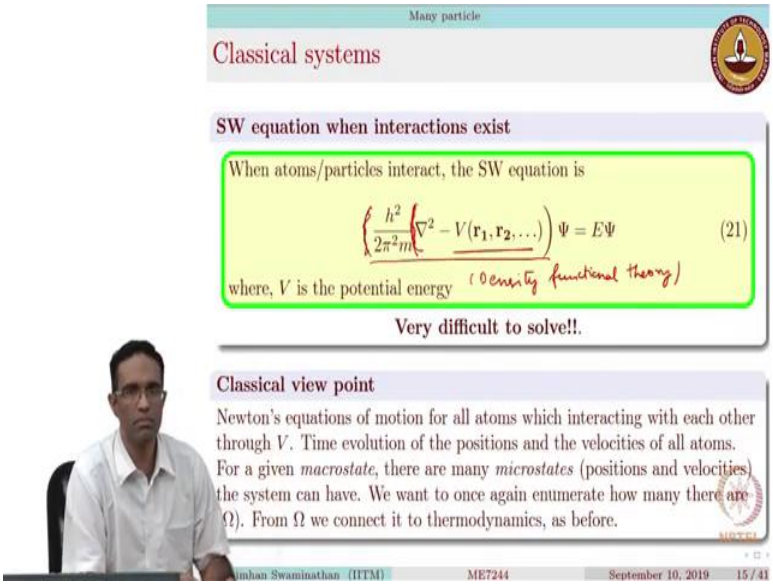

Some of you have been, have already asked me in last class; what happens when you have an interaction in system between the atoms? So, when the particles are going to interact then the Schrodinger Wave equation becomes this, so I think there should be a bracket like that. That becomes a Schrodinger Wave equation and when this potential energy is present, it becomes extremely difficult to solve the differential equation. Consequently we have to resort the numerical techniques like density functional theory and others in order to solve these equations.

But that is subject of a different, that is a different subject and that is not something that we will cover in class today. However, we do not… But it is not necessary that we need to always solve Schrodinger Wave equation. At times it is possible for us to actually resort to the classical view

point especially when we are not going to consider the contribution of electrons, then it is okay if we actually not solve the Schrodinger Wave equation but instead take a classical point of view.

So what does classic mean? Classical means you can actually solve Newton's equations in order to predict the system's behavior and not necessarily the Schrodinger Wave equation. So, in Newton's equation of motion, all the atoms are basically, so the manner in which it is done is as follows, so you consider a system compromising of a large number of atoms and each of these atoms are actually interacting with each other through some force field, through some potential.

And you can write down equations of motion for each, every particle comprising the system and consequently when you solve the equations of motions, you get the positions and the velocities of all the atoms compromising the system as a function of time.

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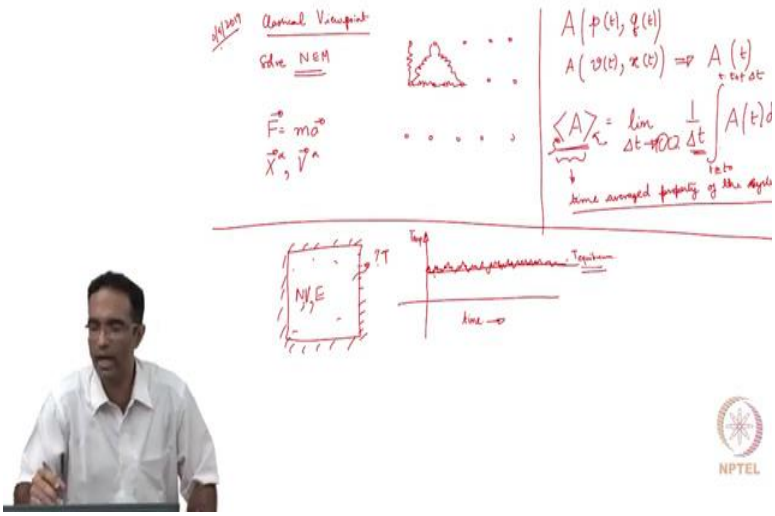


So, classical viewpoint, solve Newton's equations of motion, that is it. So, you have a large number of atoms and they are all interacting with each other through some spring, through some non-linear springs. We do not know what these, we do not know the functional form of these springs yet, they are all interacting with each other. And given some initial positions for all these atoms, some initial velocities for all these atoms you can solve F equal to ma.

And as a result of this you will get the positions, position vector and the velocity vector for all the atoms comprising of the system. The basic idea in classical statistical thermodynamics, the

classic statistical mechanics is that – all the properties, any property, any property say A of the system is actually a function of the momentum and positions of the system. So, I am intentionally using p and q which are always used whenever we talk about classical systems.

We do not only talk about velocities and positions, rather we talk about generalized momenta and generalized positions and we will see the, we will I will give you some examples as to why there is usually powerful. So, you for a time being you can view this as say the velocity of the system, of all the particles in the system, and the positions of all the particles in the system. So, I know the A, I know a functional form for this property A as a function of velocity and a position of all the particles in the system.

Consequently it also is a function of time, which means I know it as a function of time because the positions and the velocity are now revolving as functions of time when we solve the equations of motion. So, once I know this property A as a function of time, then I can calculate the time averaged property of the system using something like this. So, this is actually the time averaged property of a system.

Student: what is delta t tending to ?

Professor: Infinity, a very large number, infinity. Now do you have any questions? Do you want to question this?

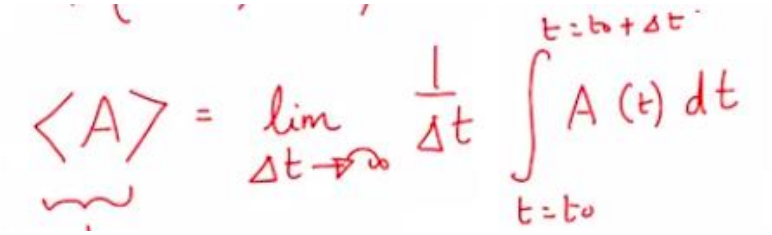
Student: what is delta t tending to ?

Professor: What is now? That day also that is the first question I am expecting. What is this, what is infinity, what is delta t? What is this property? What are these brackets? Time average, it is called time averaging or, as we will see in a little bit it is also called as, can be, can also be used to a present something called as the ensemble averaging.

The whole idea here is that when you are talking about a system in equilibrium, its temperature does not change. For example, if you have a system, the system that we saw which was constrained in particles, volume V and energy E was held fixed for this particular system. What is its temperature? Is it temperature upon? Yes?

Student: Is t not divided by delta…?

Professor: Yes. We should divide it by delta.



So we are actually looking for this quantity. Once you know this quantity you know what, that, so let me motivate this by looking at this isolated system here. You have large number of atoms and they are constrained to be, it is an isolated system, its volume is constrained, the number of particles is constrained and the energy is fixed, the matter of state is fixed.

Now, the question that we ask is – What is a temperature of a system? So, the answer to that is if you actually take the temperature of the system and plot it as a function of time, it is going to be looking something like this. It is going to be fluctuating about the value that it is going to have at equilibrium. It is not going to be a fixed number. It is going to be fluctuating above some value that it will have at equilibrium. And it so happens that this fluctuations or these vibration, this time scale is going to be in the order of, what is the order of vibrations of atoms, what is the frequency? Maybe 10 to the power…

Student: 12 or 13

Professor: 12, 13 hertz, 10 to the power 13 hertz, the atoms are vibrating at very high frequency, so the, if you average this over even a reasonable time, say it for example, in the order of 100 pico second, a few 1000 pico seconds also, it averages out and it gives you the equilibrium temperature that the system is going to have with very little error.

So, when you are putting a thermometer and trying to measure the temperature of a system, the temperature that you are actually measuring is the value that it has averaged out over that small time over which you have fixed it and because these vibrations… vibrations of the atoms happen at such high frequencies, the value that you are reading off of it gives you the right equilibrium value that it is going to have from it at equilibrium.

So, this delta t is actually not very large number, large mean compared to 1 second. It is very-very small time. That time is actually infinity enough for us to actually calculate these quantities in general, unless you are looking, if you are looking at temperature it is enough that there are certain other quantities where this may not be enough, we talk about it later.

But for quantities such as pressure, temperature, especially there are solids, such approximations are good enough, a few 100 pico seconds will give you a reasonable averaging of the property that you are looking for, but that is not the case when you talk about discuss liquids and polymers and things like that because the relaxation time for these materials is much large, we will talk about it when we come to it. But then, did you get the whole idea as to why we are performing this time average.

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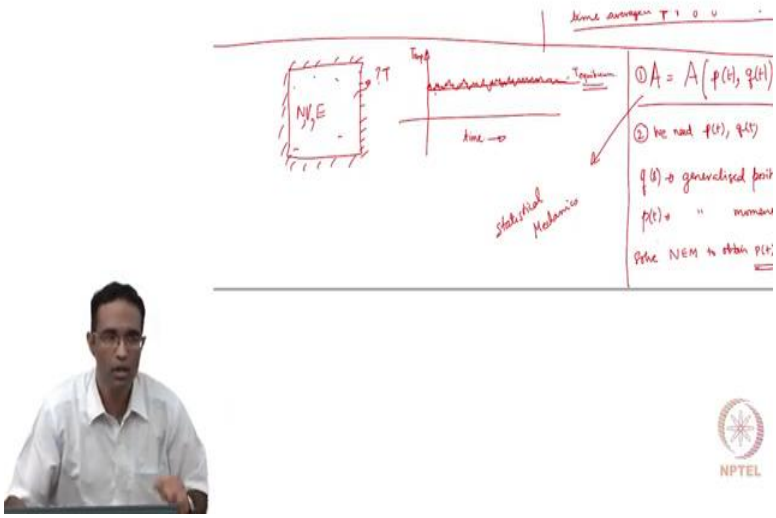

So, the two things have appeared here. one is the fact that we need to know what this a is as a function of momentum and the position. We need to know the explicit functional form, for example, if we are talking about pressure, how is pressure a function of the position and the velocity of all the atoms, we need to know that or else we need to know how the Gibb's free energy is a function of positions and velocities of all the atoms.

If we know that, then we can take the average of it overtime to calculate what its, you know, what its value is going to be at equilibrium. The second thing is, we need p of t and q of t, which

is basically the evolution, time evolution of the position and the momentum. q is generally used to generalized position. ... momentum. How do we obtain this p of t and q of t?

By solving Newton's equations, theoretically we can solve Newton's equations of motion to obtain p of t and q of t. So, first we need this explicit functional form and that functional form is given by statistical mechanics and these evolution of p and q are, it is given by Newton's equations, by solving Newton's equations of motion. So, it is a good idea to actually look at how these Newton's equations of motion are written down and to illustrate a few additional concepts that is generally associated with solving these equations because they are always easy to solve.

They are easy to solve for some simple systems but for complicated systems like one atom connected to 100, 1000 other atoms is not a very easy problem to solve, even if you look at simple Newtonian mechanics. So, we have to introduce certain methodologies that you will frequently see whenever you are working with a molecular dynamic simulation, so we want to do that now.

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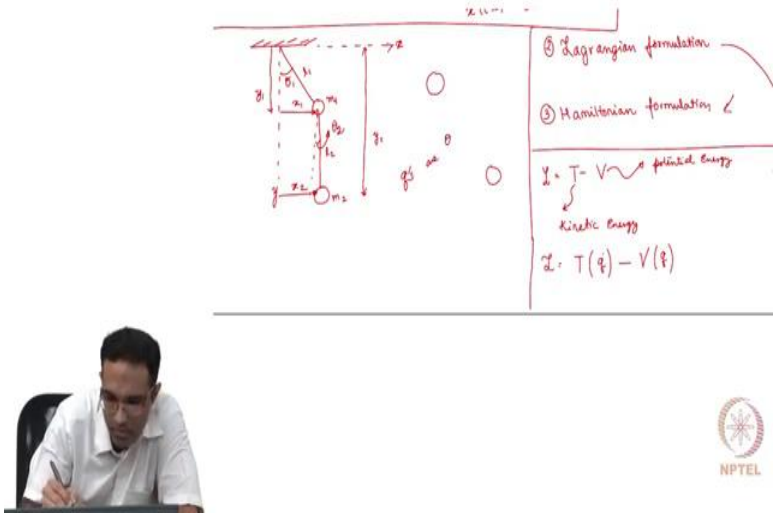
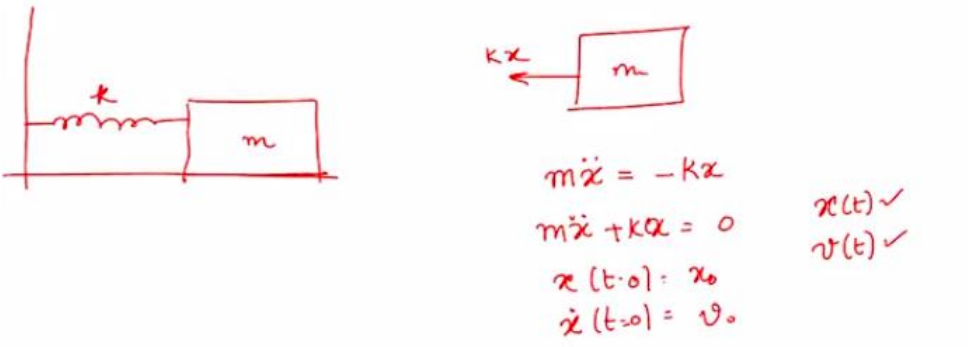


So, first of all before we solve the Newton's equations of motion we need to be able to write down the equations of motions, we need to be able to write down the equations of motions. This is generally done in several different ways, each of which has its own advantage and

disadvantage. I would like to illustrate these methods using a very simple example to show you that they all result in the same equations of motion.

You may have looked at this before when you studied classical mechanics, nonetheless I think it is a good idea to have a recap of some of that. So, I am going to take a very simple problem. The problem is that of a block which is connected mass m, is connected to a linear spring of spring constant K. This block is perturbed from its equilibrium position and left to oscillate… left to oscillate.



So, how would you write down the equations of motions for this in general? What would be the first step?

Student: free body diagram

Professor: Free body diagram. You draw free body diagram and if it being pulled to the right you would say that this is Kx, this is mass m, so the equations of motions is nothing but Mx double dot is equal to minus Kx so mx double dot plus Kx is actually equal to 0 which will essentially, which is basically a second order differential equation, so given the value of x at t equal to 0 and the velocity at t equal to 0.

You can basically predict and solve this differential equations and get x as a function of t and obviously the velocity also can be obtained as a function of t. Now, all our problems are not this simple. For example, if you take this problem where this is actually a double pendulum problem,

these lengths L1 and L2 are fixed and this is going to be my x1 and this is going to be my y1 and this is going to be my y2 and this is going to be my x2.

Now, if you write down the equations of motions like the way we did for the previous problem, you have to do it, you have to draw free body diagram of each body and then write down the equations of motion in the x direction, in the y direction for each of these two masses. In addition to that, see that there is a constraint on x1 and y1, x1 square plus y1 square, the whole group must be equal to L1 and all these things actually make the, make your derivation of the equations of motion very-very messy.

It makes it very-very complicated. You can do it and see, you know how to do this, you can do it and see how messy it gets and how hard it is to actually even write down the equations of motion correctly and then we alone solving. However, there are alternative methodologies by which you can write down the equations of motion in a very simple manner. There are two such methods one is called as the Lagrangian formulation, and what is the other one?

Student: Hamilton

Professor: What is that?

Student: Hamilton.

Professor: Hamiltonian formulation, I think we have studied before or no?

Student: No

Professor: Okay. You know these things can be, these things are not, I am not trying to convince you that if you know these whatever I have been talking for about 35 minutes, you can master Lagrangian formulation and Hamiltonian formulation, do not get me wrong. These are probably courses by themselves, to understand how you actually solve and write down these equations of motions. It is quite involved.

But you will get the essence of what these Lagrangian formulation and Hamiltonian formulation are actually doing and how easy it becomes for you to at least write down the equations of motion. And in whenever you are solve, whenever you are using molecular dynamics which is

actually one of the main part of this course. You have, you are actually solving Newton's equations of motion but first you know, you should know how to write and for complicated system you cannot expect to write summation of f x equal to ma, mx double dot, that is not the way it is done, you have to use Lagrangian formulation or Hamiltonian formulation to actually even write down the equations of motion before solving.

So, that is the reason why I think it is useful for us to know these formulations and is going to use the same block problem to show you that through the Lagrangian formulation also we will get exactly this equation and through Hamiltonian formulation also we will exactly the same equation, just to illustrate that.

So, in the Lagrangian formulation … in the Lagrangian formulation you write something called as the Lagrangian which is the difference between the kinetic and a potential energy, this is the first step.

$$\mathcal{L} = T(\dot{q}) - V(q)$$

This is the kinetic energy, this is the potential energy. So, the Lagrangian is written as a function of the generalized momenta or momenta, so ... momenta, so g as a function of the velocity and the potential is a function of the position.

I will show you an example of this through the double pendulum to know what exactly this q dots and q, they are called generalized, q is basically generalized position. For example, in the double pendulum problem, this and this are the generalized position, is not necessary for us to know x1 and y1, it is more than enough if we know what theta1 is, if you know theta of m as a function of time we can write theta one dot which is basically the velocity of this one.

We do not need to know x1 and y1 but identifying the generalized problem itself can be complicated for certain systems, that this system has actually got simple, only theta 1 and theta 2. So, you can write q, so q for the double pendulum problem are theta 1 and theta 2. So, once you know this Lagrangian, then you do the following.

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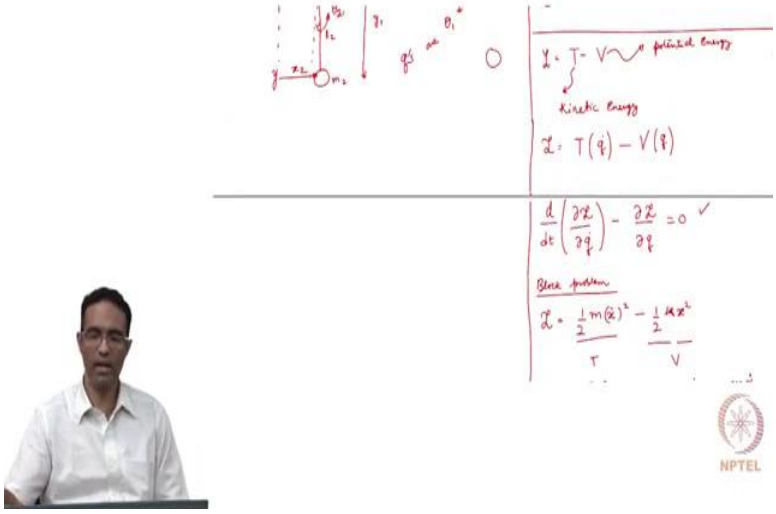
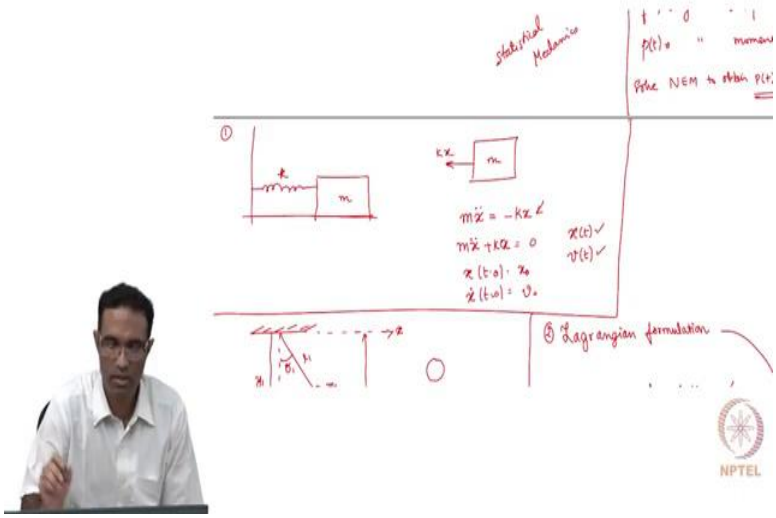




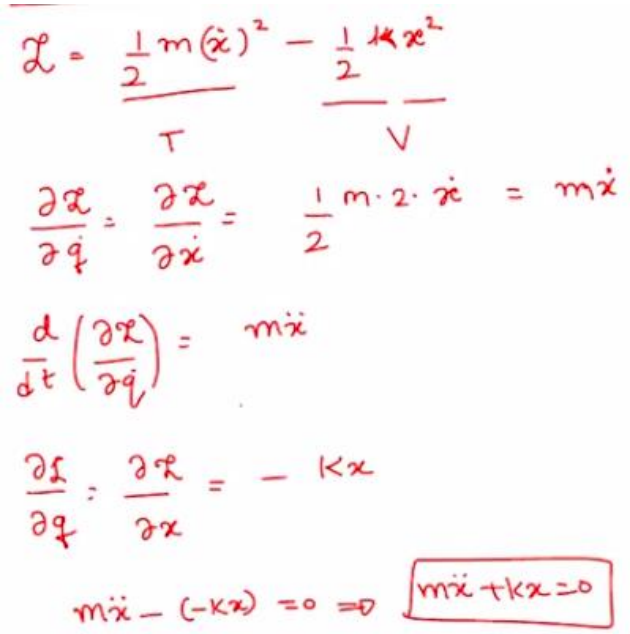
If you do this, you will get a equations of motion of any system. d by dt of dou l by dou q dot minus dou l by dou q is equal to 0 will give you the equations of motion.

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}}\right) - \frac{\partial \mathcal{L}}{\partial q} = 0$$

So, if there are many q's, if there is a qx if there are many-many q's you will do it for each one of them and you get the corresponding equations of motion for each direction and so on and so forth.

So, for our block problem, for the block problem, what is L? Assuming that q is same as x. What is L? Half m x dot square minus half K, half K x square. This is T and this is V. Now, let us do, let us perform these operations here. What is dou l by dou q dot and what is d by dt of? And dou L by dou q is nothing but dou L by dou x which is nothing but minus kx.

So, when I substitute this in the, in this expression right here, and this expression right here, I get mx double dot minus of minus kx is equal to 0.



And this is exactly the same as what we got here. And this is not the total energy, this is actually something T minus V is basically called the Lagrangian, the difference between the kinetic and the potential energy, it is not the total energy. We need to remember that.

So, this is another matter by which you can actually get the equations of motion. This is in much more, this methodology becomes much more powerful and clear when we actually try to solve the double pendulum problem. So, I have a link here in my slides.

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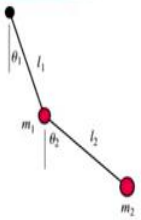
Double Pendulum



A double pendulum consists of one pendulum attached to another. Double pendula are an example of a simple physical system which can chaotic behavior. Consider a double bob pendulum with masses m_1 and m_2 attached by rigid massless wires of lengths l_1 and l_2

Further, let the angles the two wires make with the vertical be denoted θ_1 and θ_2, as illustrated above. Finally, let gravity be given by g.

the positions of the bobs are given by

$$x_2 = l_1 \sin\theta_1 + l_2 \sin\theta_2$$
$$y_2 = -l_1 \cos\theta_1 - l_2 \cos\theta_2.$$

The potential energy of the system is then given by

$$V = m_1 g y_1 + m_2 g y_2$$
$$= -(m_1 + m_2) g l_1 \cos\theta_1 - m_2 g l_2 \cos\theta_2,$$

and the kinetic energy by

$$T = \tfrac{1}{2} m_1 v_1^2 + \tfrac{1}{2} m_2 v_2^2$$
$$= \tfrac{1}{2} m_1 l_1^2 \dot{\theta}_1^2 + \tfrac{1}{2} m_2 [l_1^2 \dot{\theta}_1^2 + l_2^2 \dot{\theta}_2^2 + 2 l_1 l_2 \dot{\theta}_1 \dot{\theta}_2 \cos(\theta_1 - \theta_2)].$$

The Lagrangian is then

$$L \equiv T - V$$
$$= \tfrac{1}{2}(m_1 + m_2) l_1^2 \dot{\theta}_1^2 + \tfrac{1}{2} m_2 l_2^2 \dot{\theta}_2^2 + m_2 l_1 l_2 \dot{\theta}_1 \dot{\theta}_2 \cos(\theta_1 - \theta_2)$$
$$+ (m_1 + m_2) g l_1 \cos\theta_1 + m_2 g l_2 \cos$$

and the kinetic energy by

$$T = \frac{1}{2}m_1 v_1^2 + \frac{1}{2}m_2 v_2^2$$

$$= \frac{1}{2}m_1 l_1^2 \dot{\theta}_1^2 + \frac{1}{2}m_2[l_1^2\dot{\theta}_1^2 + l_2^2\dot{\theta}_2^2 + 2l_1 l_2 \dot{\theta}_1\dot{\theta}_2 \cos(\theta_1 - \theta_2)].$$

The Lagrangian is then

$$L \equiv T - V$$

$$= \frac{1}{2}(m_1 + m_2)l_1^2\dot{\theta}_1^2 + \frac{1}{2}m_2 l_2^2\dot{\theta}_2^2 + m_2 l_1 l_2 \dot{\theta}_1\dot{\theta}_2 \cos(\theta_1 - \theta_2)$$

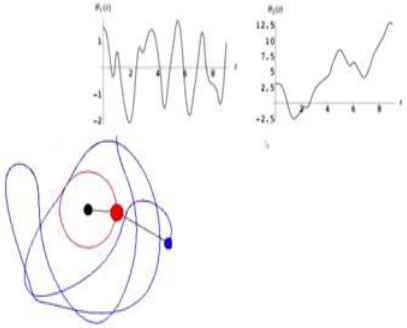
$$+(m_1 + m_2)gl_1 \cos\theta_1 + m_2 g l_2 \cos$$

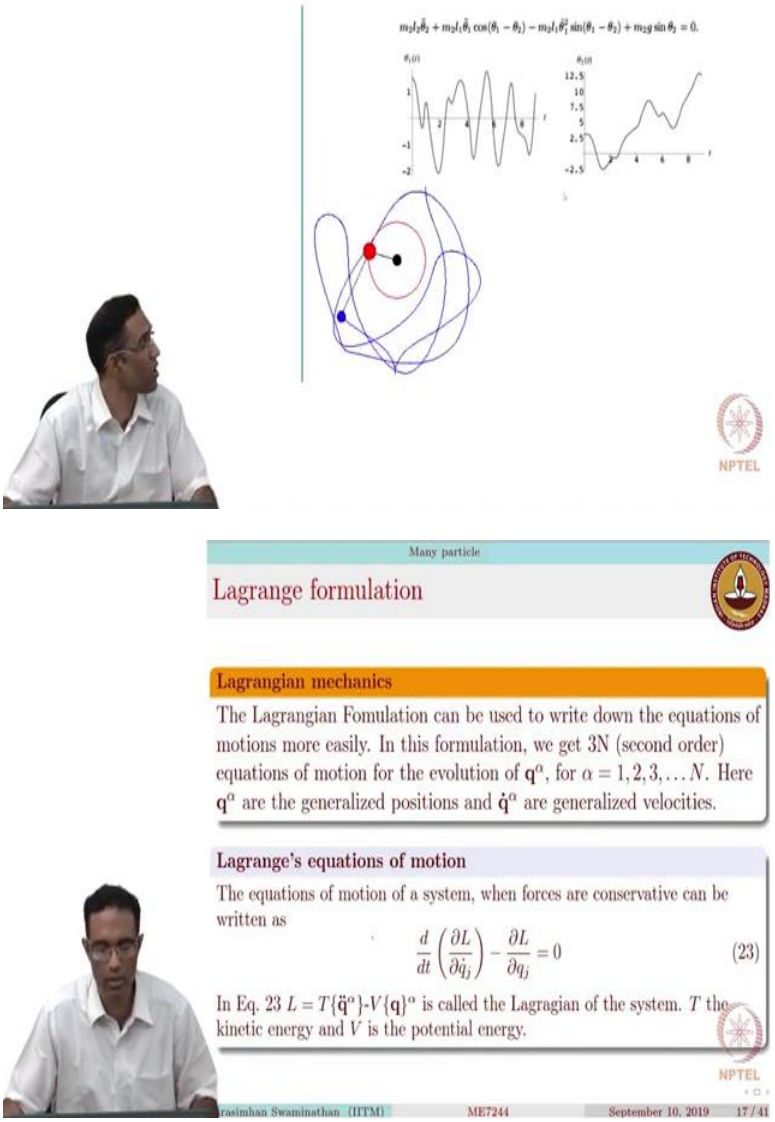
Therefore, for θ_1 .

$$\frac{\partial L}{\partial \theta_1} = m_1 l_1^2\dot{\theta}_1 + m_2 l_1^2\dot{\theta}_1 + m_2 l_1 l_2 \dot{\theta}_2 \cos(\theta_1 - \theta_2)$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\theta}_1}\right) = (m_1 + m_2)l_1^2\ddot{\theta}_1 + m_2 l_1 l_2 \ddot{\theta}_2 \cos(\theta_1 - \theta_2) - m_2 l_1 l_2 \dot{\theta}_2 \sin(\theta_1 - \theta_2)(\dot{\theta}_1 - \dot{\theta}_2)$$

$$m_2 l_2\ddot{\theta}_2 + m_2 l_1\ddot{\theta}_1 \cos(\theta_1 - \theta_2) - m_2 l_1\dot{\theta}_1^2 \sin(\theta_1 - \theta_2) + m_2 g \sin\theta_2 = 0.$$





So, look at the double pendulum problem here. So this is from this particular website right here, so theta 1 and theta 2 are the two degrees of freedom, zoom it. Is it okay? Theta 1 and theta 2 are the two degrees of freedom right here. So I write down x1 as l1 sin theta 1 and x y1 as l minus l1 si... cos theta 1 assuming that my x is in this direction and my positive y is pointing upwards.

And same thing with x2 and y2 and now the potential energy of the system can be completely written in terms of theta 1 and theta 2. The kinetic energy also can be written completely in terms of theta 1 and theta 2. It is very-very simple, and now write down T and V and then take the Lagrangian T minus V, which is completely in terms of theta 1 dot and theta 1 and theta 2.

Now, do exactly what we did, d by dt of for theta 1, d by dt of dou l by dou theta 1 dot minus dou L by dou theta 1, it essentially give you the equation of motion, this is the entire equation of motion right here, this one. The entire equation of motion for just theta 1 and this one could be a corresponding one for theta 2, so the number of steps that we actually had to write down.

There is algebra here, there is nothing much any complicated and I will write down the equation, forget about solving, that is a different ball game altogether. But writing down the equations of motion became very simple when we actually took this approach of writing down the Lagrange and the Lagrange is actually a, it is not a vectorial quantity, it is actually a scalar quantity, it is a difference of two energies.

From the scalar quantity we are able to derive the equations of motion that is governing the system. And this is actually the double pendulum which has been solved. You can take a look at the website, this is really nice. So, now the Lagrange's equations of motion are in terms of theta double dot and therefore there are two second order differential equations which have to be solved in order to see what how theta 1 and theta 2 are varying time.

They just theta 2 double dot is basically a second order equations so you have to just solve it. So, we will not go into the solution on these equations but I just want to illustrate what these things do and how easy it is to writing equations of motion if you follow the Lagrange, if you follow the writing equation of motion through the Lagrange's method.

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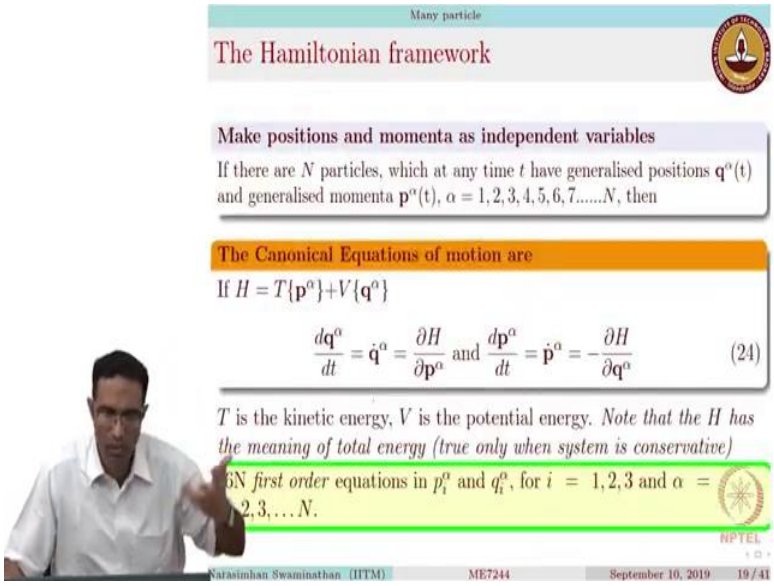

Now, there is another methodology which is called as the Hamiltonian framework in which the momenta and the positions are both covered, the momentum of each particle and the position of each particle are treated separately.

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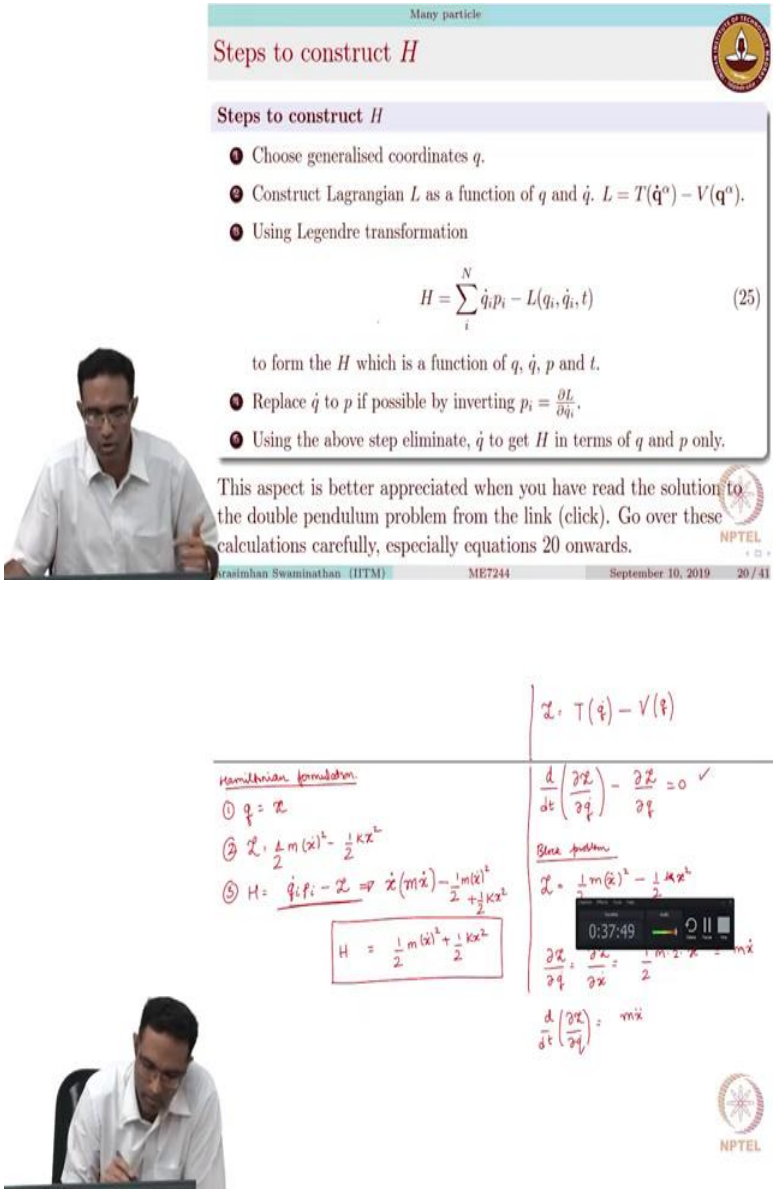


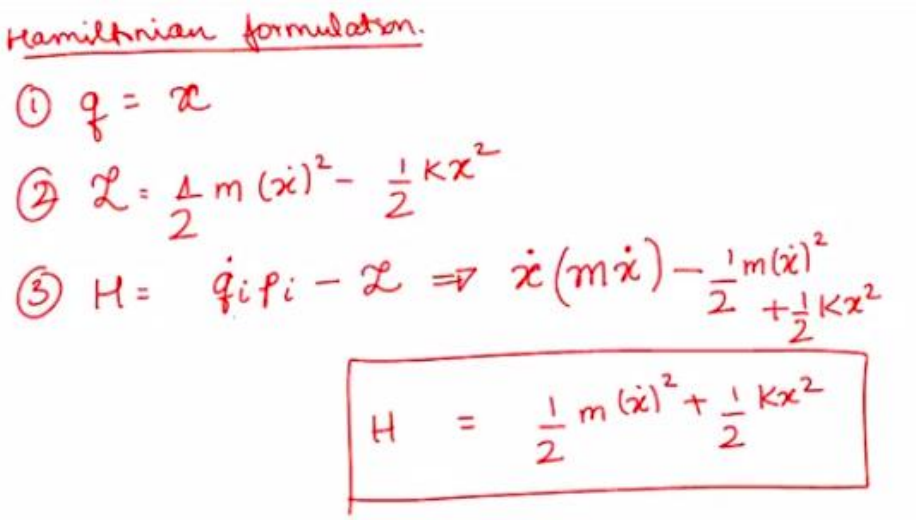
So, these are the methodologies that you actually, this is the methodology that you generally follow in order to construct what is referred to as the Hamiltonian, once you know this H, you can actually write down the equations of motion. So, we will follow these procedures and we will find out what the equations of motion are for the same block problem and see if it turns out to be the same thing as what we derived from the, from our general procedure. So, the first step is choose generalized coordinates.

So, the generalized coordinates are is just x in our case but it can be theta, like for the double pendulum problem like I just showed you. So, first step, the next step is construct Lagrangian as a function of q and q dot, so we know how to do that also which is nothing but T minus V. So, we say to construct the Lagrangian which is half m x dot square, x square.

The next step is using Lengendre transformation, construct the Hamilton, using Lengendre transformation is q i dot Pi minus L, so is nothing but q dot, q dot is nothing but x dot, Pi is nothing but the corresponding momentum minus L and this becomes… What does this become? What is this?

Student: Total energy.

Professor: Total energy of the system.



Conservatives system, if you follow this procedure carefully, the Hamilton and the total energy of the system is the same, that is why I have written it down like this, but you cannot always say that H is equal to the total energy of the system. You have to follow this procedure, you have to first write down what the generalized position is, then write down Lagrangian and perform a proper Legendre transform like that to get the Hamilton.

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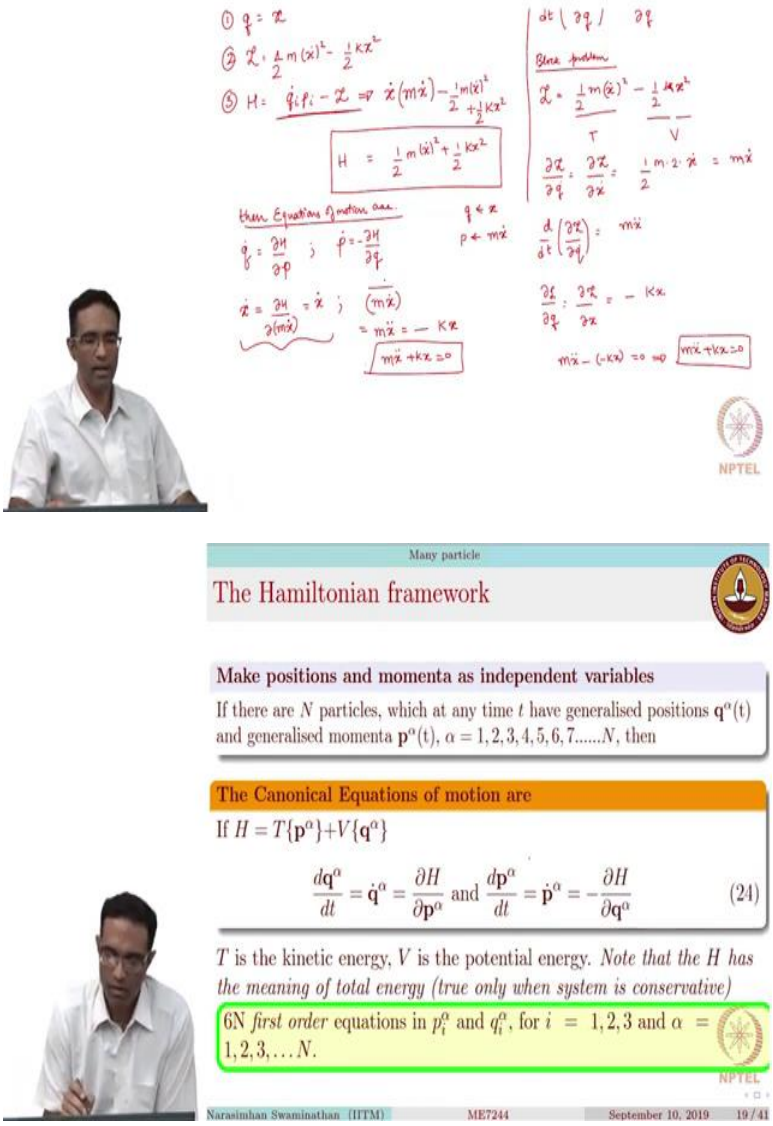
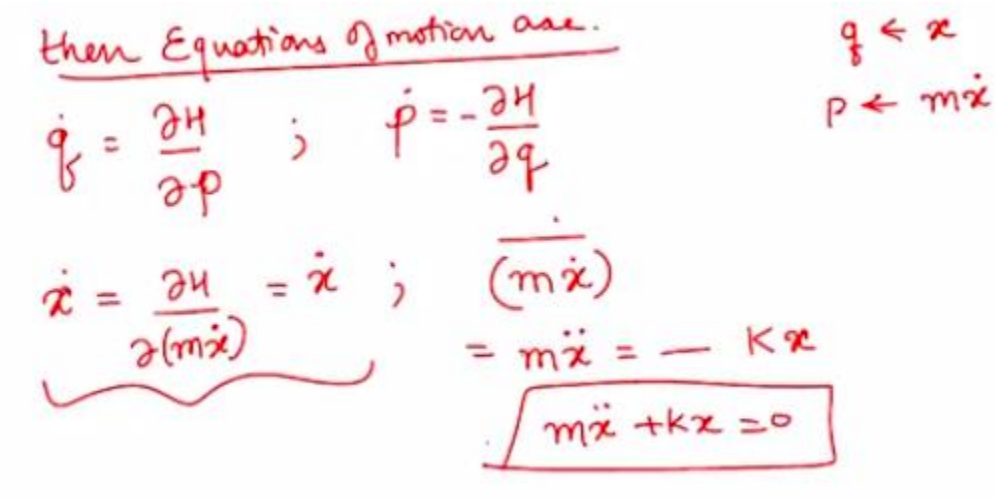


So, once you know the Hamilton, once you know H then the equations of motion are given by these. Q dot is equal to dou H by dou p, so and p dot is equal to dou H by dou q, where in our problem q is nothing but x and p is nothing but mx dot. Can you perform this differentiation to convince yourself that you get back mx double dot plus kx equal to 0?

So, in this problem so xq is nothing but x so I am saying x dot is equal to dou H by dou p, so dou H must be differentiated with respect to mx dot. So what does that give you here? It gives you

again x dot if you will, so this is kind of, in this case it is turning out to be trivial, it just says x dot equal to x dot but it will not be the case for more complicated problems.

For example, the double pendulum problem, this is not going to be the case. P dot is mx dot, the whole dot is equal to mx double dot is equal to minus of dou H by dou q which is dou x by dou x in this case, which is K times x.



I am sure you guys are thinking what is a Point? In this simple problem it does not appear to actually you have contributed much, always we were ready to get mx double dot plus Kx equal to 0 and you know this seems to be a lot of work for this specific problem.

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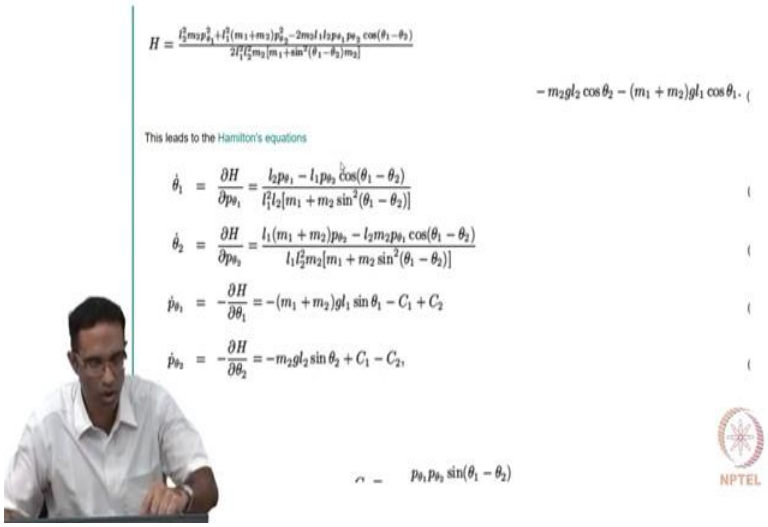

But if you look at the double pendulum problem that is not the case. You can take a look at it and if you write down the Hamilton, you will get these as the Hamilton's equation, right here: Theta 1 dot, theta 2 dot, P theta 1 dot, P theta 2 dot. For each theta 1 and theta 2 there will be corresponding momenta associated with them also.

And instead of getting second order differential equations, you get coupled first order differential equations and you treat, the positions and the momentum are treated kind of separately, and there are several other advantages which pan out by if you are using the Hamilton's formulation you know to solve differential equations or write down and solve write down the differential equations.

These things are not the focus of this class, I just want to emphasize that whenever we are doing molecular dynamics simulations we are essentially solving equations of motion and when you are solving equations of motion, the first point of starting would be the appropriate Hamilton. You have to start with H and after that only you have to derive the appropriate equations of motion for that system.

So, just to acquaint you with these terminologies Hamilton, Hamilton's equations of motion, Lagrange's equations of motion and kind of highlight some of its advantages over the regular

way of doing it, by drawing a free body diagram, we have these few examples and discussions. If you want to learn more about this you should take a course on classical mechanics.

But that will not be necessary for any of the exams or anything that you are about to do, maybe some very simple problems which should be easy to solve, without any difficulties. So, we can solve the equations of motion, we can write down the equations of motion if we follow the appropriate method, that is the basic idea of this class.

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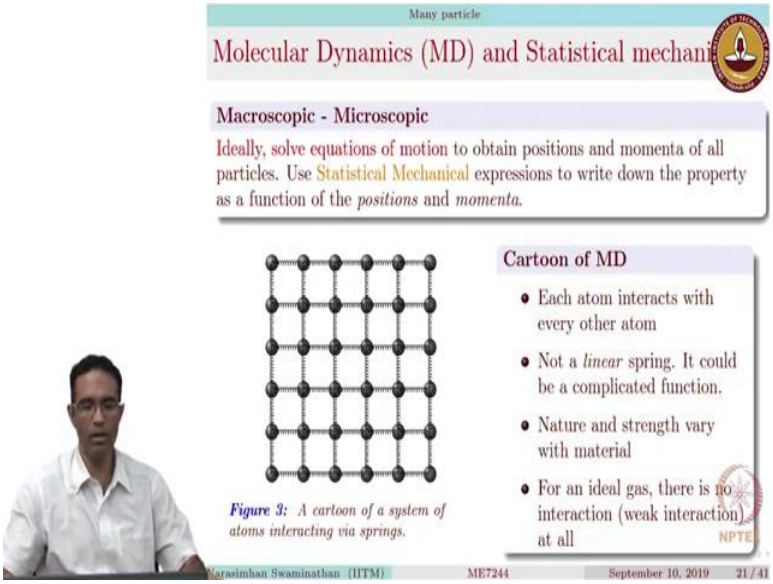

So let me just introduce this and then we will end this class. In molecular dynamic simulations, what we are doing is essentially solving the equations of motion, so we are assuming all like this with all the atoms and all of them are connected or interacting with each other. The spring should not mislead you in thinking that every atom is only interacting with its nearest neighbor, each atom could be interacting with something that is really far away and you have to solve the equations of motion, but I have always been saying solve solve, the two important things that are required for solving I have not yet talked about. What is that?

Student: initial conditions

Professor: Initial positions and initial conditions. One thing for solving I have already taught you how to do, initial positions. You know how to construct the crystal structures that is the initial position. What would be the initial velocity? We need initial velocity for all these atoms

otherwise you cannot solve the equations of motion, so from where would be initial velocities come?

Student: Temperature.

Professor: Temperature, if you knew the temperature then you can somehow assign initial velocities through all these atoms so that the temperature of the entire system is something. And that will help you solve the differential equations. Rather there is going to, that is what LAMMPS is going to do when it is solving the differential equation, it is going to take some initial velocities, some initial positions. It will start showing you these atoms oscillating over a, you know what…. a time, as a function of time. But we still need one small thing, we need to know how will the property can actually be represented as a function of these positions and the momentum. We still do not know that. We know only, we know how to involve p and q as a function of time by solving the Newton's equations.

We still do not know how any thermodynamic property can be written as a function of p and q and that is why the formalism of statistical mechanics will come in. We will talk about that in the subsequent classes. So, with that I would like to stop today's class.