Advanced Mathematical Methods for Chemistry
Prof. Madhav Ranganathan
Department of Chemistry
Indian Institute of Technology, Kanpur

Module - 10
Lecture - 01
Partial Differential Equations (PDE)

In this module I am going to talk about Partial Differential Equations. Now we have been talking about ordinary differential equations for quite a few week. Now what we will find is that many of the techniques that we use for ordinary differential equations they can be applied for partial differential equations. However, there is a fundamental difference between ordinary differential equations and partial differential equations and that is why we are will consider them separately. But what we will see is that with a few tricks you can convert partial differential equations into ordinary differential equations.

Now, before I gets before we get started discussing about partial differential equations in their solutions. Let us look at certain examples of partial differential equations that that you might have seen or you or you might be used to in various courses. So, the most probably one partial differential equation that everybody has seen in physical chemistry has to do with the Schrödinger equation and quantum mechanics.

So, suppose you have a single particle of mass m.

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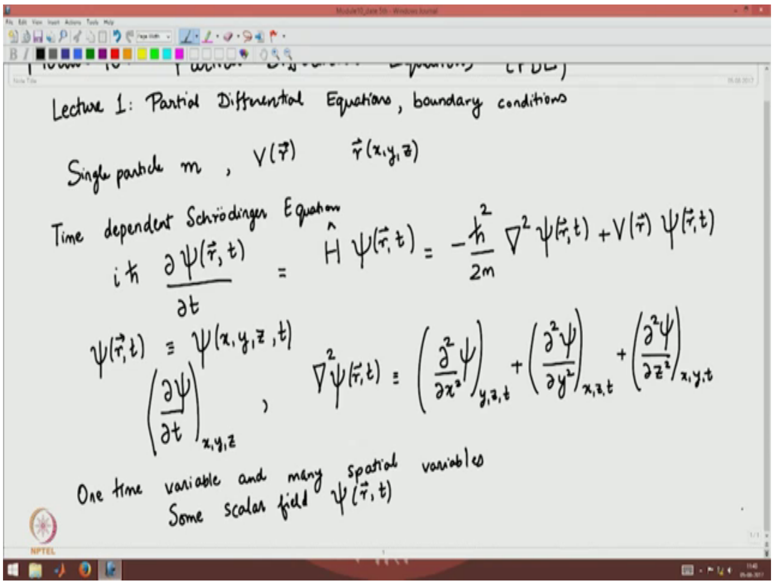

So, if you have a single particle of mass m. And it is moving in a potential V of r, r is a special coordinate. And r can have a coordinate xyz. Then the time independent Schrödinger equation or let me actually start with the time dependent Schrödinger equation, which is the equation of motion for this particle is given by is given by a dou of a function called psi which is which is called the wave function now psi is a function of r and t.

So, we write it as i H bar dou psi by dou t, is equal to an operator H of psi of r t. And now what this operator this operator is called the Hamiltonian operator and this is equal to for a single particle of mass m this is a sum of 2 terms one is the kinetic energy term, which looks like minus H cross square by 2 m Laplacian square, or this is a Laplacian del square of the gradient dotted into itself of psi of r t. And you have another term that is V, this is a potential energy of r psi of r t.

So, this is called the time dependent Schrödinger equation, and the time independent Schrödinger equation the time independent Schrödinger equation. So, here psi is a function of r and t. And that is equivalent t you can write it as a function of x y z and t. And so, when you say when you say dou psi by dou t, you are keeping you are keeping the variables x y z fixed. So, this is this is what you mean by dou psi by dou t.

Similarly, when you say when you say when you say del the Laplacian of psi del square psi. So, what this is del square you can write in Cartesian coordinates as dou square by dou x square of psi. And what you keep fixed are y z and t plus dou square psi by dou y square and now you keep x z and t fixed. And then you have dou square y dou square psi by dou z square, and here you keep x y and t fixed ok.

So, this is this is the this is the detail of this equation; however, when we write in short we will just write ih cross dou psi by dou t is equal to my is equal to this term this minus H square H cross square by 2 m del square psi plus V psi. So, this is one very common equation that you see. Notice that: that usually you have you have one time variable, and many spatial variables. The other thing that you see is that you have some field some in this case it is a scalar field psi of which is a function of both the spatial variable and the time variable.

So, there is some scalar field that depends both on the spatial variable and the time variable. So, the point I want to make is that partial differential equations or PDEs for short, are very common when working with fields.

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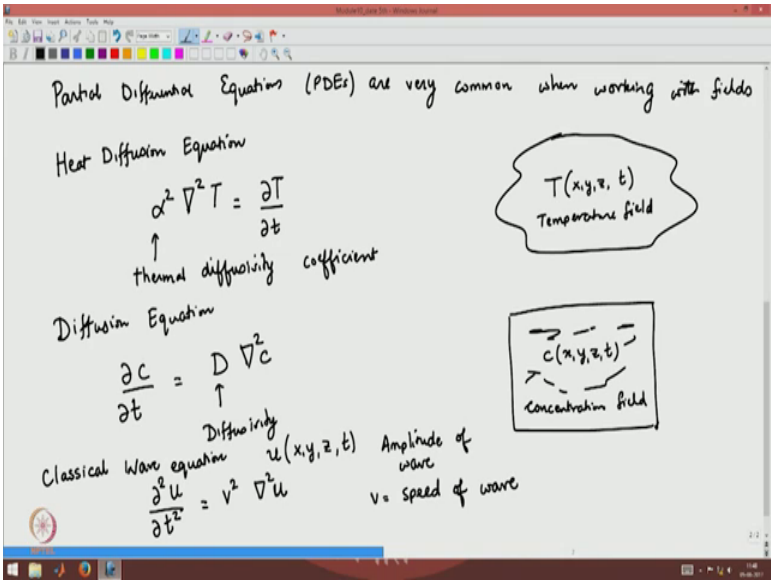

So, for example, suppose you have, suppose you have a body. So, suppose you have a body and let us say the temperature of the body is not uniform. So, temperature of the body is a function of the spatial coordinate and the time coordinate. This is a temperature field that is an example of a field ok.

So, a field is some object that as we said it is a function of spatial coordinates, and then in this case there is also time. So, you could have a temperature field. Now the partial differential equation for this is known as the as a heat equation, heat diffusion equation. That is that is given by alpha square del square t is equal to dou t by dou t. So, the heat diffusion equation is another partial differential equation, now t is a function of x y z and t. Alpha is called the is called the thermal diffusivity coefficient. Then you could also have a fields like suppose you have some region and you have you have various species in this region and there is a there is a solution, such that there is a concentration, the concentration is a function of x y z and t. This is a concentration field ok.

Then there is a there is a diffusion equation dou C by dou t and C again is a I would not I would not write the dependence is equal to D those the Laplacian of C. Now D is called the diffusivity or the diffusion coefficient. Now the point is that whenever you have a fields and you want to study the time dependence of that field typically you have some partial differential equation. There are many other examples now the other thing that I should I should mention is the is a what is called the classical wave equation ok.

Now, you have an amplitude u of a x y z t, this is the amplitude of the wave. And this usually satisfies a differential equation dou square u by dou t square is equal to Laplacian of u and there is a C, or I will just put a I will, I will, I will call it a V, V square. So, V is equal to speed of wave. So, V is the speed of the wave and so and so the classical wave equation has this form. So, these are some of the common partial differential equations that appear. Now I should I should mention a few things. So, let us get back to the Schrödinger equation. Now we wrote the Schrödinger equation in this form ok.

Now, often whenever we deal with partial differential equations.

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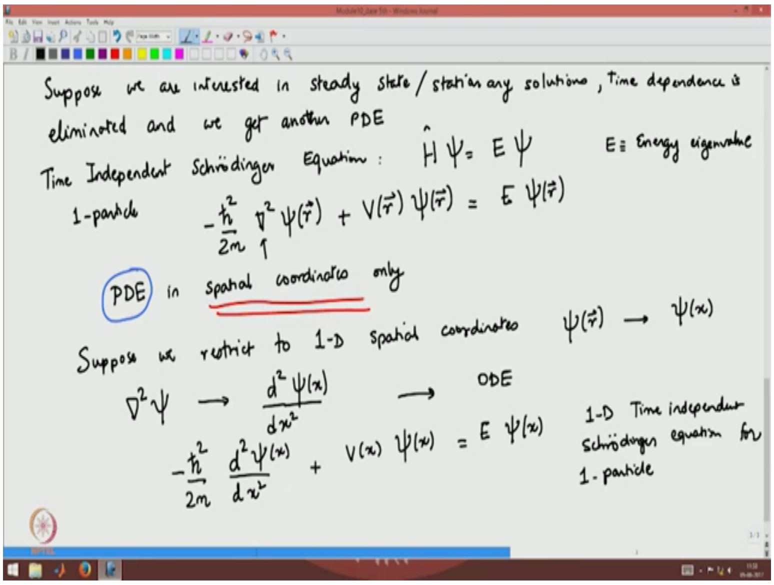

So, suppose we are interested in steady state solution slash I will say stationary solution, steady state is also called stationary solutions. So, then what happens is in the in this case the time dependence is eliminated. And we get another PDE. So, let us take the Schrödinger equation. So, the So suppose you say suppose you say you say that the time independent Schrödinger equation. This is just we can we can write this as H psi equal to E psi, E is called the energy eigenvalue. And now this for a for a one particle. This becomes minus H bar square by 2 m del square psi of r t, r now this is independent of time is plus V of r psi of r is equal to e times psi of r ok.

So, this is a this is the time independent Schrödinger equation, this is also a PDE. So, this is also a PDE because there is a there is a Laplacian here. Now so this is PDE in spatial coordinates. So, the point is the point is what is what is important here is that it is a PDE only in spatial coordinates. But it is still a PDE, but it is still a PDE it is still a PDE. It is not become an ode at. Now further suppose we suppose we restrict to 1D spatial coordinates. So, suppose you have a particle that is only allowed to go in one dimension. Then what happens is that your then del square psi becomes D square psi, well So, the first thing that happens is psi of r becomes psi of x, and this becomes D square psi by dx square.

So, this becomes an ode. So, your equation becomes an ode and that equation for a particle that is allowed to move only in one dimension becomes this form, plus V of x psi of x is equal to e times psi of x. So, this is a this is a 1 dimensional time independent Schrödinger equation, equation for one particle; so for one particle moving with this external potential V of x. So, the lesson that I want to mention is that is that when we look for stationary solution you can you can get rid of the time independence. And when you get rid of the time independence you still have a PDE. And that PDE unless you have a 1 dimensional problem it does not become an ode.

So, the heat diffusion equation has this form now suppose the temperature is suppose the temperature reaches a steady state then this heat diffusion equation has this form. So, steady state Heat equation.

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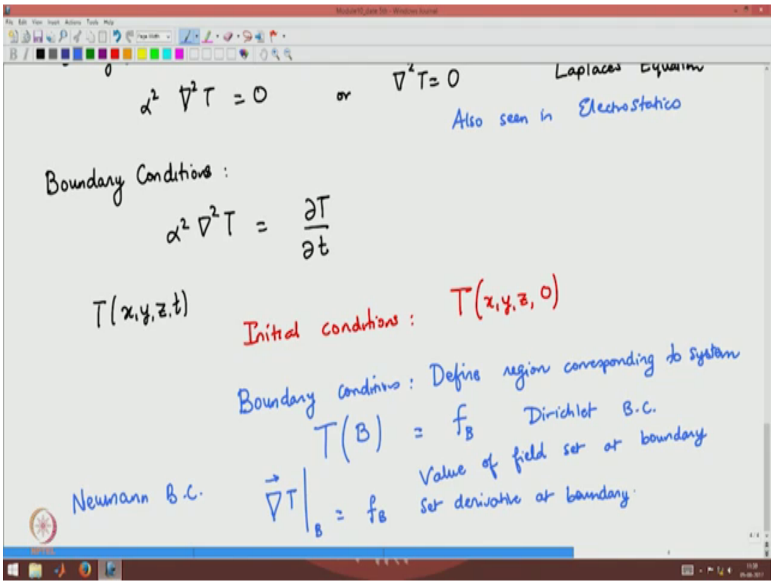

This is this is basically alpha square del square t equal to 0 or del square t equal to 0. This is called the Laplace's equation, again it is a it is a very common equation, we also see this equation in electrostatics. So, this is also seen in electrostatics. In fact, in fact Laplace's equation is one of the very common partial differential equation. And of course, if you have it in one dimension then you just get D square t by dx square equal to 0.

One of the one of the most interesting things about partial differential equation is, is that is the boundary conditions; so usually a PDE. So, for example, let us take the heat equation. Now as we said there are t is a function of xyz and t. So, you can have 2 kinds of boundary conditions you can have what are called as initial conditions. For example, you could have t of xyz at 0, and you could have you could have some initial conditions either on the first derivative or the second derivative whichever. So, then you could have then you could have what are called as boundary conditions. So, the boundary conditions involved they you need to define region corresponding to system ok.

So, you define the spatial region corresponding to the system and you define when you put boundary conditions on the system. So, you could have the temperature evaluated at whatever the boundary is so the boundary I will just say B. And this is usually it is you might set it to some value. So, the temperature at the boundary is I will just call it f B. So, this is this sort of boundary condition where the value is set the boundary is called a

Dirichlet boundary condition. So, value of field set at boundary. So, you set the value you could also have what are called as Neumann boundary conditions or noiman boundary conditions, which is a gradient of t at boundary is equal to some value. So, set derivative at boundaries ok.

So, these are the kind of boundary conditions that you can have, and what we will see is that is that the Domain of p of PDE or the region of or the spatial region of PDE.

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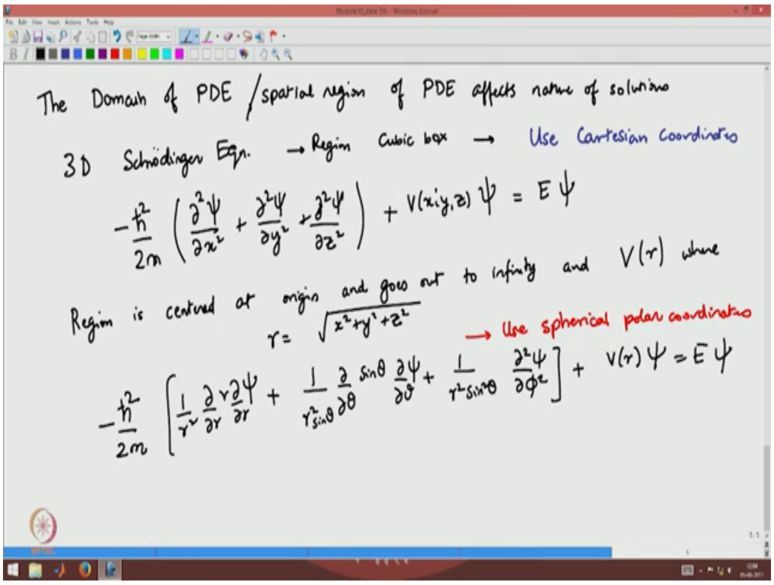

So, whatever the way you define the spatial region where the PDE is applicable, that is what decides the nature of the solutions. So, this affects nature of solutions. So, the most simple example is you can take you can take the 3 dimensional Schrödinger equation, now if you had if your if your region was a was a cubic box.

So, let us take a 3 D Schrödinger equation, if your region was a cubic box. So, region cubic box, then you typically writes the equation in Cartesian coordinates. So, there you use Cartesian coordinates. Now in this case you get your equation becomes dou square psi of psi is a function of xyz. So, just write dou square psi by dou x square plus dou square psi by dou y square plus dou square psi by dou z square, this is equal to plus V of xyz psi is equal to E psi. Now you it looks like it looks like a second order partial differential equation in each of these variables

Now, on the other hand if your region, is let us say centered at a origin and goes out to infinity. And V is written as a function of r. So, V is written as a function of r, where r is equal to square root of x square plus y square plus z square. Now in this case you are in this case you are going to use spherical polar coordinates. And so and so, you are Schrödinger equation will you will have to write the Laplacian in spherical polar coordinates. So, you will have one over r square dou by dou r of r dou by dou r, and then you will have a r square dou by dou theta of sin theta dou by dou theta r square sin theta. And you will have another term one over r square sin square theta dou square by dou psi square, ok.

So, now your psi is a function of r theta phi plus V which is a function only of r psi equal to E psi. So, now, notice that this differential equation looks very different. So, here it nicely separated into xyz, but here the r term and theta term are all are all you know and the and the phi term they all seem to be mixed with each other. So, the point is this will have very different solutions and this. And what we will see in the next few lectures is how to how to take the partial differential equations apply these boundary conditions and try to solve for whatever the quantity of interest is.

I will conclude this lecture here. So, in the next lecture we look at we look at the common methods to or we look at one very common method that is used to solve partial differential equations.

Thank you.