Ordinary Differential Equations

CHEM 361B: Introduction to Physical Chemistry

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Lecture 2

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Learning Objective: Practice the math required to solve quantum mechanical systems

Differential Equations (DE) - Classification

An ordinary DE is when functions of one independent variable exist

$$L\frac{d^2Q(t)}{dt^2} + R\frac{dQ(t)}{dt} + \frac{1}{C}Q(t) = E(t)$$

A partial DE is when functions of more than one independent variable exist

$$\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial^2 y} = 0$$

The order of a DE is the order of the highest derivative that appears.

For example, the order of the two above equations is two.

DEs - Classification (cont.)

A DE is said to be linear if it is a linear function of the variables y, y',...,$y^{(n)}$. This would take the form of

$$a_0(t)y^{(n)} + a_1(t)y^{(n-1)} + \cdots + a_n(t)y = g(t)$$

An equation not of this form is said to be nonlinear. For instance, the DE for an oscillating pendulum

$$\frac{d^2\theta}{dt^2} + \frac{g}{L}\sin\theta = 0$$

is nonlinear.

DE Review - Solving a Simple First Order ODE

A first order linear ODE can take the form of

$$\frac{dy}{dt} + p(t)y = q(t)$$

and these are separable if

$$f(y)dy + g(t)dt = 0$$

It is solved by integrating both sides. For a complete description, an initial condition needs to be specified.

An Example of Solving a First Order DEs

Find the solution for

$2\frac{dy}{dx} + 6y = 4; \qquad y(0) = 2$

Second Order DEs

A second order linear DE takes the form of

$$\frac{d^2y}{dt^2} + p(t)\frac{dy}{dt} + q(t)y = g(t)$$

but we are first going to look at a particularly simple example:

$$\frac{d^2y}{dt^2} - y = 0$$

where taking the derivative twice of the function gives the function back.

Solving Second Order DEs

Two solutions to this DE emerge

$$\begin{aligned} y(x) &= c_1 e^x \\ \frac{d}{dx} c_1 e^x &= c_1 e^x \\ \frac{d}{dx} c_1 e^x &= c_1 e^x \end{aligned}$$

$$\begin{aligned} y(x) &= c_2 e^{-x} \\ \frac{d}{dx} c_2 e^{-x} &= -c_2 e^{-x} \\ \frac{d}{dx}\left(-c_2 e^{-x}\right) &= c_2 e^{-x} \end{aligned}$$

as well as the sum of these two solutions

$$\begin{aligned} y(x) &= c_1 e^x + c_2 e^{-x} \\ \frac{d}{dx}\left(c_1 e^x + c_2 e^{-x}\right) &= c_1 e^x - c_2 e^{-x} \\ \frac{d}{dx}\left(c_1 e^x - c_2 e^{-x}\right) &= c_1 e^x + c_2 e^{-x} \end{aligned}$$

Solving Second Order DEs (cont.)

Returning to a more general Second Order DE

$$a\frac{d^2y}{dt^2} + b\frac{dy}{dt} + cy = 0$$

if we use the general solution se^{rt} to solve this we get:

$$s(ar^2 + br + c)e^{rt} = 0$$

This implies that

$$(ar^2 + br + c) = 0$$

where r is determined by solving for zeros and any constants (s) are determined from the initial conditions.

A Second Order DE Example

Solve the following DE

$\frac{d^2y}{dt^2} - \beta^2 y = 0, \quad y(0) = 0, \quad y'(0) = 1$

Summary

- The order of the differential equation is the order of the highest derivative that appears in the equation
- In this course, we will explicitly solve second order differential equations where the solution will have the form $y = se^{rt}$