ENGINEERING PHYSICS

R Vasudevan Iyer, Ph.D.

Department of Science and Humanities

Concept of Hamiltonian operator

Class #21

- The kinetic energy and potential energy operators are $\hat{K} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ and $\hat{V}$
- Since sum of kinetic and potential energies is the total energy E we have E = K + V
- If K and V are treated as operators then the sum of them is also an operator. Thus $\hat{E} = \hat{K} + \hat{V}$
- The total energy operator is referred to as the Hamiltonian operator and is written as $\hat{H}$. Thus $\hat{H} = \hat{K} + \hat{V} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \hat{V}$
- The Hamiltonian can also be written as the time operator, $\hat{H} = i\hbar\frac{\partial}{\partial t}$

One dimensional Schrodinger's time dependent equation

PES UNIVERSITY ONLINE

- We know that quantum systems are described by the wavefunction,ψ
- Quantum systems would undergo changes as time progresses. For example the electron in an atom changes its position, momentum, energy etc with time as it interacts with the environment.
- This change must manifest itself as changes in the wavefunction and thus ψ must change with time
- How do we monitor such a change?
- This was first shown by Erwin Schrondinger and the equation showing time evolution of a quantum system is known as the Schrodinger's time dependent equation.

One dimensional Schrodinger's time dependent equation

- We start with the equation E = K + V
- The physical quantities are now treated as operators and we write an operator equation, $\hat{E} = \hat{K} + \hat{V}$
- We apply the operators to the wavefunction of the quantum system as follows: $\hat{E}\Psi = \hat{K}\Psi + \hat{V}\Psi$
- The operators are now written in their mathematical form which then leads to $i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + \hat{V}\Psi$. Note that we still have not defined the operator corresponding to the potential energy. We will elucidate this point later
- The equation shown is the famous Schrodinger's equation and is written in the concise form as $\hat{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t}$

One dimensional Schrodinger's time dependent equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + \hat{V}\Psi$$

- we note that the Schrodinger's time dependent equation has a first order derivative in time and second order derivative in space
- The unique feature of this equation is the presence of i. If not for i this equation would resemble the heat equation. Due to the presence of i it becomes an equation representing the flow of probability
- It is a partial differential equation.
- As it is linear if ψ_1 is a solution to this equation and ψ_2 another independent solution then $a\psi_1 + b\psi_2$ is also a solution. This has deep significance

One dimensional Schrodinger's time dependent equation

- We will come across quantum systems where the potential energy is a function of space only (V(x)).
- Also in many quantum systems the total energy for a given state remains constant (E = constant)
- When we consider these two aspects we ask the question – how does the Schrodinger's equation change.
- To see what changes will happen we take the time dependent equation try to solve it

One dimensional Schrodinger's time dependent equation

- To solve a partial differential equation we make use of a technique called SEPARATION OF VARIABLES
- We assume that the wavefunction, Ψ, which is a function of space and time, can be written as $\Psi(x,t) = \psi(x)f(t)$
- We now substitute this in the equation $i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + \hat{V}\Psi$

  to get $i\hbar\frac{\partial\psi f}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi f}{\partial x^2} + \hat{V}\psi f$
- In the LHS we see that the derivative is w.r.t time and hence we write it as

$$\psi\left(i\hbar\frac{df}{dt}\right) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi f}{\partial x^2} + \hat{V}\psi f$$

One dimensional Schrodinger's time dependent equation

- In RHS we note that the first term is a derivative of space. In the second term we see that then potential energy operator acts on the wave function. We have chosen systems where potential energy is a function of space only and hence any mathematical form representing the potential energy operator must act on functions of space only.
- Thus we have $\psi\left(i\hbar\frac{df}{dt}\right) = f\left(-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \hat{V}\psi\right)$
- Also note that we change from partial derivatives to total derivatives

One dimensional Schrodinger's time dependent equation

- Continuing further we make the following changes $\frac{1}{f}\left(i\hbar\frac{df}{dt}\right) =$

$$\frac{1}{\psi}\left(-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \hat{V}\psi\right)$$

- Now note that LHS is a function of time only whereas the RHS is a function of space only. If they have to be equated then both have to be equal to some constant. Let us call the constant as G (referred to as separation constant)

- Thus $\frac{1}{f}\left(i\hbar\frac{df}{dt}\right) =$ G and $\frac{1}{\psi}\left(-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \hat{V}\psi\right) = G$

One dimensional Schrodinger's time dependent equation

- Solving for LHS we get $f = Ae^{-\frac{i}{\hbar}Gt}$. Generally one form of the wave function is $\Psi = Ae^{\frac{i}{\hbar}(px-Et)}$. This can be written as $\Psi = Ae^{\frac{i}{\hbar}(px)}e^{-\frac{i}{\hbar}Et}$
- We see a pattern . The time behaviour is always has the form $e^{-\frac{i}{\hbar}Et}$. The space behaviour in this case is $\psi = e^{\frac{i}{\hbar}(px)}$ whereas in a general case is denoted by $\psi(x)$. Hence for behaviour of quantum system is always represented by $\Psi = \psi(x)e^{-\frac{i}{\hbar}Et}$. We immediately see that the separation constant is the total energy E which we have taken to be constant.

One dimensional Schrodinger's time dependent equation

- Thus we have $\frac{1}{\psi}\left(-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\hat{V}\psi\right)=E$
- The obvious question now is what mathematical representation can we assign to $\hat{V}$?
- In all the situations we will come across we have the following: V = 0 or V = V_0 or V = V(x). Therefore our potential energy operator is simply V. We cannot ascribe any mathematical form to it.
- Hence we have $\frac{1}{\psi}\left(-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V\psi\right)=E$ which can be written as $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V\psi=E\psi$. This is one dimensional Schrodinger's time independent equation.

One dimensional Schrodinger's time dependent equation

- The equation can be written as $\hat{H}\psi = E\psi$ the eigen value equation.
- Therefore when we solve the Schrodinger's time independent equation we are solving the eigen value equation to obtain the eigen value E and the eigen function ψ
- Most of the time the Schrodinger's equation is presented as $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$
- The 1D Schrodinger's time independent is an ordinary linear differential equation and as before

Class #21 …….. Quiz….

- If ψ_1 is a solution to the time independent Schrodinger's equation and ψ_2 another independent solution then which of the following is true?.
- $a\psi_1 + b\psi_2$ is also a solution
- $a\psi_1 + b\psi_2$ is not a solution
- $ab\psi_1\psi_2$ is also a solution
- $a\psi_1 / b\psi_2$ is also a solution

THANK YOU

R Vasudevan Iyer, Ph.D.

Professor, Department of Science and Humanities

rviyer@pes.edu