

Free Study Material from All Lab Experiments



Quantum Mechanics & Applications
Chapter - 1
Time Dependent Schrodinger Equation

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Time Dependent Schrodinger Equation

Syllabus: Time dependent Schrodinger equation and dynamical evolution of a quantum state; Properties of Wave Function. Interpretation of Wave Function Probability and probability current densities in three dimensions; Conditions for physical Acceptability of Wave Functions. Normalization. Linearity and Superposition Principles. Eigen-values and Eigen-functions. Positions, momentum and Energy operators; commutator of position and momentum operators; Expectation values of position and momentum. Wave Function of Free Particle. alllabexperiments.com

Q.1. State briefly the basic postulates of Quantum Mechanics?

Ans. The postulates of QM are given below: Support by Donating

- **Postulate 1:** The state of a system is described completely in terms of a state vector $\psi(r,t)$ which is quadratically integrable.
- **Postulate 2:** To every physically observable there exist a linear hermitian operator.
- **Postulate 3:** In any measurement of the observable associated with \hat{A} operator the only value that will ever be observed are the eigenvalue a_i , which satisfy the eigenvalue equation $\hat{A}g_i = a_i g_i$.
- **Postulate 4:** The eigen functions of operators corresponding to observable forms a complete set.
- **Postulate 5:** If a system is in a state described by a normalized wave function ψ , then the average value of the observable corresponding to \hat{A} is given by $\langle A \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{A} \Psi dr$.
- **Postulate 6:** The wave function or state function of a system evolves in time according to the time-dependent schrodinger equation

$$H\Psi(r,t) = i\hbar \frac{\partial \Psi}{\partial t}$$

Q.2. Derive time dependant Schrodinger wave equation? Also discuss how quantum states evolve with time?

Ans. Let a particle wave of wave function

$$\Psi(x,t) = Ae^{i(kx - \omega t)} \quad (3)$$

For a free particle of momentum $p = \hbar k$ and energy $E = \hbar \omega$. With this in mind, we can then note that

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 \Psi \quad \text{alllabexperiments.com} \quad \dots(1)$$

Which can be written, using $E = p^2 / 2m = \hbar^2 k^2 / 2m$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = \frac{p^2}{2m} \Psi \quad \dots(2)$$

Similarly
$$\frac{\partial \Psi}{\partial t} = -i\omega \Psi \quad \dots(3)$$

Which can be written, using $E = \hbar \omega$:

$$i\hbar \frac{\partial \Psi}{\partial t} = \hbar \omega \Psi = E \Psi \quad \dots(4)$$

We now generalize this to the situation in which there is both a kinetic energy and a potential energy then, $E = p^2 / 2m + V(x)$ so that

$$E \Psi = \frac{p^2}{2m} \Psi + V(x) \Psi \quad \dots(5)$$

Where Ψ is now the wave function of a particle moving in the presence of a potential $V(x)$. But if we assume that the results Eq.(2) and Eq.(4) still apply in this case then we have

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x) \Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad \dots(6)$$

Which is the famous time dependent schrodinger wave equation. It is setting up and solving this equation, then analyzing the physical contents of its solution that form the basis of that branch of quantum mechanics known as wave mechanics.

In general, the solutions to the dependent schrodinger equation will describe the dynamical behaviour of the particle, in some sense similar to the way that Newton's equation $F=ma$ describes the dynamics of a particle in classical physics.

Q. 3. What is the physical interpretation of wave function (ψ), wave function probability and probability current density?

Ans. If there is a wave associated with a particle, then there must be a function to represent it. This function is called wave function.

Wave function is defined as that quantity whose variations make up matter waves. It is represented by Greek symbol Ψ (psi), Ψ consists of real and imaginary parts.

$$\Psi = A + iB$$

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Physical Significance of Wave Functions (Born's Interpretation)

Born's interpretation

The wave function Ψ itself has no physical significance but the square of its absolute magnitude $|\Psi|^2$ has significance when evaluated at a particular point and at a particular time $|\Psi|^2$ gives the probability of finding the particle there at that time.

The wave function $\Psi(x,t)$ is a quantity such that the product

$$P(x,t) = \Psi^*(x,t)\Psi(x,t)$$

Is the probability per unit length of finding the particle at the position x at time t .

$P(x,t)$ is the probability density and $\Psi^*(x,t)$ is complex Ψ conjugate (x,t)

Hence the probability of finding the particle is large wherever Ψ is large and vice-versa.

Probability Current Density - In quantum mechanics, the probability current (sometimes called probability flux) is a mathematical quantity describing the flow of probability in terms of probability per unit time per unit area.

We have proposed that $|\Psi(x,t)|^2$ is a probability density

$$P(x,t) = |\Psi(x,t)|^2 \quad \dots(2)$$

much like the fluid number density. The time derivative of this probability is then:

$$\frac{\partial P}{\partial t} = \frac{\partial(\Psi^* \Psi)}{\partial t} = \Psi \left(\frac{\partial \Psi^*}{\partial t} \right) + \Psi^* \left(\frac{\partial \Psi}{\partial t} \right) \quad \dots(3)$$

Where we have dropped the arguments from the wave function Ψ . The one-dimensional Schrodinger equation provides what we need for the second term on the RHS, and its complex conjugate

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$$-i\hbar \frac{\partial \Psi^*(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi^*(x,t)}{\partial x^2}$$

Provides the first term. Substituting,

$$\frac{\partial P}{\partial t} = \frac{1}{i\hbar} \left(\frac{\hbar^2}{2m} \Psi \frac{\partial^2 \Psi^*}{\partial x^2} - \frac{\hbar^2}{2m} \Psi^* \frac{\partial^2 \Psi}{\partial x^2} \right)$$

$$\text{alllabexperiments.com} \quad = -\frac{1}{i\hbar} \frac{\hbar^2}{2m} \frac{\partial}{\partial x} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right)$$

Note the choice of bonus signs. This has the same functional form as the equation of continuity,

$$\partial P / \partial t = -\partial j / \partial x$$

its just a question of defining the probability current j (same as the flux f , but for probability). It should be clear from the derivative on the RHS that the correspondence is

$$j = \frac{\hbar}{2im} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right)$$

Q. 4. What are the basic conditions of function to be a wavefunction?

Ans. NORMALIZATION CONDITION

The probability per unit length the particle at position x at time is

$$P = \psi^*(x,t)\psi(x,t)$$

so, probability of finding the particle in the length dx is

$$Pdx = \psi^*(x,t)\psi(x,t)dx$$

Total probability of finding the particle somewhere along x -axis is

$$\int Pdx = \int \psi^*(x,t)\psi(x,t)dx$$

If the particle exists, it must be somewhere on the x -axis. So the total probability of finding the particle must be unity i.e.

$$\int \psi^*(x,t)\psi(x,t)dx = 1 \quad (1)$$

This is called the normalization condition. So a wave function $\psi(x,t)$ is said to be normalized if it satisfies this condition.

ORTHOGONAL WAVE FUNCTIONS

Consider two different wave ψ_m functions and ψ_n such that both satisfies Schrodinger equation. These two wave functions are said to be orthogonal if they satisfy the conditions.

$$\text{Or} \quad \int \psi_n^*(x,t)\psi_m(x,t)dv = 0 \text{ for } n \neq m \quad (1)$$

$$\int \psi_n^*(x,t)\psi_m(x,t)dv = 0 \text{ for } m \neq n]$$

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If both the wave functions are simultaneously normal then

$$\int \psi_m \psi_m^* dv = 1 = \int \psi_n \psi_n^* dv \quad (2)$$

ORTHONORMAL WAVE FUNCTIONS:

The sets of wave functions, which are both normalized as well as orthogonal are called orthonormal wave functions.

Equations (1) and (2) are collectively written as

$$\int \psi_m^* \psi_n dv = \begin{cases} 0 & \text{if } m \neq n \\ 1 & \text{if } m = n \end{cases}$$

Q.5. Describe linearity and superposition principle for a wave function?

Ans. The linearity of a Schrodinger's wave function

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t} \quad \text{alllabexperiments.com}$$

stand for-

Linearity in $\Psi(x, t)$: A linear combination $\Psi(x,t)$ of two solution $\Psi_1(x,t)$ and $\Psi_2(x,t)$ is also a solution. $c_1\Psi_1(x, t) + c_2\Psi_2(x, t)$

$\Psi_1(x,t)$ is a solution and thus satisfied

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_1(x,t)}{\partial x^2} + V(x,t)\Psi_1(x,t) = i\hbar \frac{\partial \Psi_1(x,t)}{\partial t}$$

$\Psi_2(x,t)$ is a solution and thus satisfied:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_2(x,t)}{\partial x^2} + V(x,t)\Psi_2(x,t) = i\hbar \frac{\partial \Psi_2(x,t)}{\partial t}$$

Add Eqs. E_1 and E_2 together as $c_1 E_1 + c_2 E_2$

$$\begin{aligned} & c_1 \left[-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_1(x,t)}{\partial x^2} + V(x,t)\Psi_1(x,t) \right] + c_2 \left[-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi_2(x,t)}{\partial x^2} + V(x,t)\Psi_2(x,t) \right] \\ &= c_1 \left[i\hbar \frac{\partial \Psi_1(x,t)}{\partial t} \right] + c_2 \left[i\hbar \frac{\partial \Psi_2(x,t)}{\partial t} \right] \end{aligned}$$

Rearrange a bit:

$$\begin{aligned} & -\frac{\hbar^2}{2m} \left[c_1 \frac{\partial^2 \Psi_1(x,t)}{\partial x^2} + c_2 \frac{\partial^2 \Psi_2(x,t)}{\partial x^2} \right] + V(x,t)[c_1\Psi_1(x,t) + c_2\Psi_2(x,t)] \\ &= i\hbar \left[c_1 \frac{\partial \Psi_1(x,t)}{\partial t} + c_2 \frac{\partial \Psi_2(x,t)}{\partial t} \right] \end{aligned}$$

Differentiation is linear.

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} [c_1\Psi_1(x,t) + c_2\Psi_2(x,t)] + V(x,t)[c_1\Psi_1(x,t) + c_2\Psi_2(x,t)]$$

Support by Donating $= i\hbar \frac{\partial}{\partial t} [c_1\Psi_1(x,t) + c_2\Psi_2(x,t)]$

Substitute Eqn. E_3 to recover the schrodinger equation for $\Psi(x,t)$ thus showing that $\Psi(x,t)$ is also a solution.

$$\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t}$$

Any wave function can be written as a linear combination of eigen functions of any operator.

$$\Psi(x) = c_1\Psi_1(x) + c_2\Psi_2(x) + c_3\Psi_3(x) + \dots$$

As any wave equation, the time-dependent schrodinger equation is also linear in the field Ψ variable and therefore satisfies the superposition principle. Within this context, this means that any wave functions solution of this equation can be linearly decomposed (at any time) as a sum of a series of other solution of the same equation (for the same potential function),

$$\Psi(r,t) = \sum_{i=1}^N c_i \Psi_i(r,t), \quad \dots(2.2)$$

each Ψ_i is a state whose probability of occurrence is c_i^2 . The Ψ state is made by superposition of all Ψ_i states.

Q 6. What are eigenvalue and eigenfunctions and describe the position, momentum and Energy operators with example?

Ans. The wave function for a given physical system contains the measurable information about the system. To obtain specific values for physical parameters, for example energy, you operate on the wavefunction with the quantum mechanical operator associated with that parameter. The operator associated with energy is the Hamiltonian and the operation on the wave functions the schrodinger equation. Solutions exist for the time independent schrodinger equation only for certain values of energy, and these values are called eigen values of energy.

Corresponding to each eigenvalue is an "eigenfunction" The solution to the schrodinger equation for a given energy E_i involves also finding the specific Ψ_i function which describes that energy state. The solution of the time independent schrodinger equation takes the form

$$H_{op}\Psi_i = E_i\Psi_i$$

The eigenvalue concept is not limited to energy. When applied to a general operator Q , it can take the form

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$$Q_{op}\psi_i = q_i\psi_i$$

operator eigenvalue eigenfunction

if the ψ_i functions an eigenfunction for that operator. The eigenvalues q_i may be discrete, and in such cases we can say that the physical variable is “quantized” and that the index i plays the role of a “quantum number” which characterizes that state.

Energy eigenvalues

“Eigenvalue” comes from the German “Eigenwert” which means proper or characteristic value. “Eigenfunction” is from “Eigenfunktion” meaning “proper or characteristic function”.

All operator quantum mechanics can be constructed from the basic operators for position and moment.

$$\hat{x}\psi = x \times \psi$$

$$\hat{p}_x\psi = -i\hbar \frac{\partial}{\partial x} \psi$$

For a particle in 1-dimension, we have the kinetic energy operator derived as follows:

$$\hat{T} = \frac{\hat{p}_x^2}{2m} = \frac{\hat{p}_x \cdot \hat{p}_x}{2m} = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2}$$

For a single particle moving in 1-dimensions in a potential $V(x)$, the Hamiltonian operator is given by

$$\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$$

In 3-D, we can write

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$$\hat{H} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(r) = -\frac{\hbar^2}{2m} \nabla^2 + V(r)$$

The angular momentum operator is given by-

We have already defined the operators \hat{x} and \hat{p} associated respectively to the position and the momentum of a particle. Therefore we can define the operator-

$$\hat{L} = \hat{x} \times \hat{p},$$

Then we get -

$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right), \hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right), \hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

Q 7. What is a commutator? Write its properties.

Operators (or variables in quantum mechanics) do not necessarily commute. We can see our first example of that now that we have a few operators. We define the commutator to be

$$[\hat{p}, \hat{x}] \equiv \hat{p}\hat{x} - \hat{x}\hat{p} \quad \text{alllabexperiments.com}$$

We will now compute the commutator between \hat{p} and \hat{x} . Because \hat{p} is represented by a differential operator-

$$[\hat{p}, \hat{x}]\psi(x) = \hat{p}\hat{x}\psi(x) - \hat{x}\hat{p}\psi(x) = \frac{\hbar}{i}\frac{\partial}{\partial x}\hat{x}\psi(x) - \hat{x}\frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x)$$

$$[\hat{p}, \hat{x}]\psi(x) = \frac{\hbar}{i}\left(\psi(x) + \hat{x}\frac{\partial\psi(x)}{\partial x} - x\frac{\partial\psi(x)}{\partial x}\right) = \frac{\hbar}{i}\psi(x)$$

So, removing the $\psi(x)$ we used for computational purposes, we get the commutator.

$$[\hat{p}, \hat{x}] = \frac{\hbar}{i} = -i\hbar \text{ or } [\hat{x}, \hat{p}] = i\hbar$$

Similarly for angular momentum -

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z, [\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x, [[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$$

and

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

Q 8. What is the meaning of expectation value? Give example to get the expectation value of position and momentum using any wavefunction.

Expectation Values - Operators allow us to compute the expectation value of some physical quantity given by the wavefunction. If a particle is in the state $\psi(x, t)$, the normal way to compute the expectation value of $f(x)$ is-

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} \psi^*(x)f(x)\psi(x)dx$$

If the variable we wish to compute the expectation value of (like \hat{p}) is not a simple function of x , let its operator act on $\psi(x)$. The expectation value of in the state ψ is -

$$\langle p \rangle = \langle \psi | p | \psi \rangle = \int_{-\infty}^{\infty} \psi^*(x)\hat{p}\psi(x)dx$$

This is solved example of expectation value of momentum when a particle is in a box of length L , whose normalized wave function ψ is $(2/L)^{1/2} \sin(\pi x/L)$

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$$\begin{aligned}
 \langle p \rangle &= \int_0^L \Psi^* \hat{p} \Psi dx \\
 &= \frac{2}{L} \int_0^L \sin\left(\frac{\pi x}{L}\right) \left(\frac{\hbar}{i} \frac{d}{dx}\right) \sin\left(\frac{\pi x}{L}\right) dx \\
 &= \frac{2\hbar\pi}{L^2 i} \int_0^L \sin\left(\frac{\pi x}{L}\right) \cos\left(\frac{\pi x}{L}\right) dx \\
 &= \frac{2\hbar}{Li} \int_0^L \sin\left(\frac{\pi x}{L}\right) \cos\left(\frac{\pi x}{L}\right) d\left(\frac{\pi x}{L}\right) = 0
 \end{aligned}$$

Hence the average momentum of particle in a box is zero.

Q.9. What is a free particle? Write down its wave function.

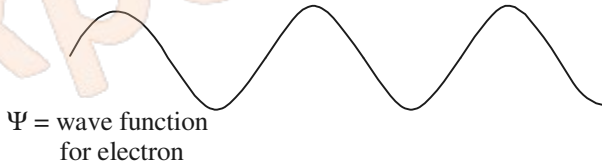
Ans. In physics, a free particle is a particle that, in some sense, is not bound by an external force, or equivalently not in a region where its potential energy varies. A free particle in quantum mechanics is described by the free Schrödinger equation in which $V(x) = 0$

$$-\frac{\hbar^2}{2m} \frac{d^2 \Psi}{dx^2} = E \Psi$$

$$\frac{d^2 \Psi}{dx^2} = -K^2 \Psi, \text{ where } k \equiv \sqrt{\frac{2mE}{\hbar^2}}$$

$$\Psi(x) = A e^{ikx} + B e^{-ikx}$$

$$\Psi(x, t) = A e^{ik(x - \frac{\hbar k}{2m}t)} + B e^{-ik(x + \frac{\hbar k}{2m}t)}$$



$$\begin{aligned}
 \Psi &= A \cos\left(\frac{2\pi}{\lambda} x - \omega t\right) \\
 &\xrightarrow{\text{Using the de Broglie relationship}} \frac{2\pi}{\lambda} = \frac{2\pi p}{h} = k \quad \text{p = electron momentum} \\
 &\xrightarrow{\text{Using the Planck relationship}} \omega = \frac{\hbar \omega}{\hbar} = \frac{E}{\hbar} \quad \text{E = electron energy}
 \end{aligned}$$



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