

for the induced magnetic field around a circular path of radius $r < R$. Assume the electric field within the plates to be uniform without any edge effect. Evaluate \vec{B} for $r = R = 55 \text{ mm}$ and $\frac{dE}{dt} = 1.5 \times 10^{12} \text{ V/ms}$. (5) [BL5]

[Hints: Use Maxwell's equations.]

5. TEM wave of frequency 300 GHz propagates in vacuum along the +ve X-direction. It has an electric field of amplitude 28.28 m. The wave is linearly polarized with the plane of vibration of the electric field at an angle 45° to the X-Z plane. Evaluate the expression of \vec{E} and \vec{B} . (10) [BL5]

[Hint: TEM wave propagates along X-direction. So $E_x = 0$, $B_x = 0$]

Module – 5 : Quantum Mechanics

Quantum Mechanical Wave Functions and Operators.

In Quantum Mechanics we can associate a wavefunction ψ with every particle. All observables in Quantum Mechanics (for example Energy, Momentum and Position) can be represented as operators. An operator has to be Hermitian in order to qualify to be a Quantum Mechanical Operator.

Following table shows different operators corresponding to different observables,

Observable	Observable	Operator	Operator
Name	Symbol	Symbol	Operation
Position	$\underline{\mathbf{r}}$	$\hat{\mathbf{r}}$	Multiply by $\underline{\mathbf{r}}$
Momentum	\mathbf{P}	$\hat{\mathbf{P}}$	$-i\hbar \left(\hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z} \right)$
Kinetic energy	T	\hat{T}	$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$
Potential energy	$V(\mathbf{r})$	$\hat{V}(\mathbf{r})$	Multiply by $V(\mathbf{r})$
Total energy	E	\hat{H}	$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V(\mathbf{r})$
Angular momentum	l_x	\hat{l}_x	$-i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$
	l_y	\hat{l}_y	$-i\hbar \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$
	l_z	\hat{l}_z	$-i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$

- The **commutative law** does not generally hold for operators. In general, $\hat{A}\hat{B} \neq \hat{B}\hat{A}$
- It is convenient to define the quantity $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ which is called the **commutator** of \hat{A} and \hat{B} .
- Note that the order matters, so that, $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$. If \hat{A} and \hat{B} happen to commute, Then $[\hat{A}, \hat{B}] = 0$. For two physical quantities to be simultaneously observable, their operator representations must commute.
- Some useful rules for evaluating commutators,

$$[\hat{A} + \hat{B}, \hat{C}] = [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}]$$

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$$

$$[\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$$

$$[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$$

- The non-commutivity of the position and the momentum operators (the inability to simultaneously determine particles position and its momentum) is represented with the Heisenberg uncertainty principle, which in mathematical form is expressed as:

$$(\Delta x)(\Delta p_x) \geq \frac{\hbar}{2}$$

- **Expectation Values.**

Any observable in quantum mechanics is represented by an operator (as mentioned earlier). Evaluation of expectation values involve Quantum Mechanical Averaging of such operators to get the average value of the corresponding observables. The expectation value $\langle A \rangle$ in terms of the wavefunction Ψ and corresponding operator \hat{A} is given by,

$$\langle A \rangle = \frac{\int_{-\infty}^{\infty} \Psi^* \hat{A} \Psi d\tau}{\int_{-\infty}^{\infty} \Psi^* \Psi d\tau}.$$

- **Particle in a one dimensional infinite potential well.**

A particle is subjected to a potential:

$$V(x) = \begin{cases} \infty, & x \leq 0 \\ 0 & 0 < x < L \\ \infty & x \geq L \end{cases}$$

After solution of the corresponding Time-Independent Schrödinger Equation the wavefunction corresponding to the n^{th} Eigen state $\psi_n(x)$ is of the form:

For $0 < x < L$

$$\psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right) \quad \text{where } n = 1, 2, 3, \dots$$

The corresponding Energy Eigen value is:.

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \hbar^2}{8mL^2}$$

Quantum Linear Harmonic Oscillator

The Quantum Linear Harmonic Oscillator like a Classical Harmonic Oscillator is subjected to a potential $V(x) = (1/2)m\omega^2 x^2$. So, the corresponding Time Independent Schrödinger Equation is:

$$\left[\frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \right] \psi(x) = E \psi(x), \quad \omega \text{ being the angular frequency of oscillation.}$$

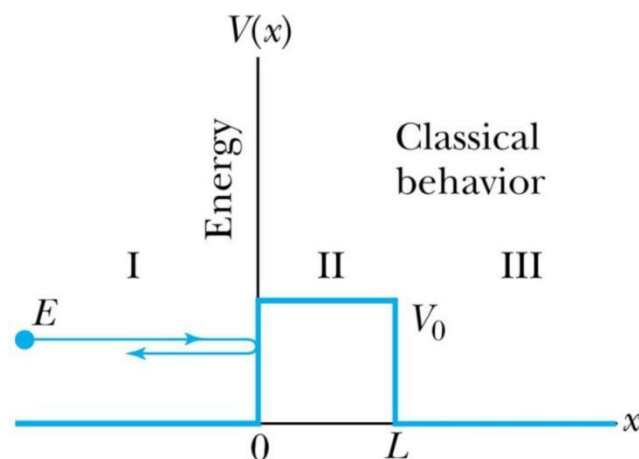
Solving the second order differential equation the energy eigen values are:

$$E_n = \hbar \left(n + \frac{1}{2} \right) \omega.$$

n is an integer. The wave functions corresponding to the eigen states are products of a Special Function known as Hermite Polynomial and a Gaussian Function.

Quantum-Mechanical Tunneling:

- Now we consider the situation where classically the particle does not have enough energy to surmount the potential barrier, $E < V_0$.
- Tunneling is a quantum mechanical phenomenon when a particle is able to penetrate through a potential energy barrier that is higher in energy than the particle's kinetic energy.



- The quantum mechanical result, however, is one of the most remarkable features of modern physics, and there is ample experimental proof of its existence. There is a small, but finite,

probability that the particle can penetrate the barrier and even emerge on the other side.

- This amazing property of microscopic particles play important roles in explaining several physical phenomena including radioactive decay. Additionally, the principle of tunneling leads to the development of Scanning Tunneling Microscope (STM) which had a profound impact on chemical, biological and material science research.
- Approximate tunneling probability $\approx \exp \left[\frac{-2\omega}{\hbar} \sqrt{2m(U - E)} \right]$

Questions:

1. Considering the ground state of a linear harmonic oscillator, find the relation between the expectation value of kinetic and potential energies. **(5) [BL4]**

[**Hint:** If calculated correctly the average values of kinetic and potential energies should be equal]

2. i) Evaluate whether the following states are eigen states of the momentum operator?
 - a) Eigen states of particle confined in a one dimensional potential well
 - b) Ground state eigen function of a simple harmonic oscillator
 - c) Ground state eigen function of a hydrogen atom
 - d) Free particle eigen function
 - e) Eigen states of particle confined in a three dimensional potential well

Justify your answer through appropriate calculation. **(5) [BL 4]**

[**Hint:** Use the expression for momentum operator and act it on the specified eigen states]

- ii) Consider a physical system which has a number of observables that are represented by the following matrix:

$$\tilde{A} = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 1 & 2 \\ 0 & 2 & 1 \end{pmatrix}$$

Find the results of the measurement of the observables. **(5) [BL4]**

[**Hint:** Evaluate the eigen values of the matrices].

3. A particle in the infinite square well has an initial wave function an even mixture of the ground and first excited states : $\psi(x,0) = A[\psi_0(x) + \psi_1(x)]$
 - a) Normalize $\psi(x, 0)$ (**Hint:** Use the orthogonality condition of the states).
 - b) Find $\psi(x, t)$ and $|\psi(x, t)|^2$ [**Hint:** Let $\omega = \frac{\pi^2 \hbar^2}{2ma^2}$]
 - c) Compute $\langle x \rangle$ and $\langle p \rangle$. Notice that $\langle x \rangle$ oscillates in time. Compute the amplitude of oscillation.
 - d) If one measures the energy of the particle, then what values are obtained? What is the probability of getting each of them? **(10) [BL4]**
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4. (a) Prove the following commutator identity :

$$[AB, C] = A [B, C] + [A, C] B \quad (5) \text{ [BL5]}$$

- (b) Using the above identity formulate that $[x^n, p] = i\hbar n x^{n-1}$ (5) [BL5]

[Hint: Apply the concept of commutator and using the knowledge of position and momentum operator derive the above relation]

5. Quantum phenomena are often negligible in the “macroscopic” world. Show this numerically for the following cases:

(a) The amplitude of the zero-point oscillation for a pendulum of length $l = 1$ m and mass $m = 1$ kg.

(b) The diffraction of a tennis ball of mass $m = 0.1$ kg moving at a speed $w = 0.5$ m/sec by a window of size 1×1.5 m².

(c) Calculate the de Broglie wavelength of the tennis ball first and using it calculate diffraction angles in the horizontal and the vertical directions.] (10) [BL5]

[Hint: (a) Apply the energy relation of the harmonic oscillator gives the average potential energy as

$$\langle V \rangle = \frac{E}{2} \text{ or } \frac{1}{2} m \omega^2 A^2 = \frac{\hbar \omega}{4} \text{ and calculate } A \text{ from this.}$$

6. Consider a particle which can move freely within rectangular box of dimensions $a \times b \times c$ with impenetrable walls. The potential can be written mathematically as;

$$V = 0 \text{ (Inside)}$$

$$= \text{infinite (at surface and outside).}$$

(a) Calculate the wave function and Energy values using Schrodinger wave equation.

(b) What do you understand about the degeneracy of the energy states? Show that for a cubical box no degeneracy is observed for the ground state, whereas first excited state is three fold degenerate? (10) [BL5]

[Hints: Apply the concept of 1D box in 3D case and using the knowledge of degeneracy calculate it.]

7. Let's suppose a particle of mass m is confined within a symmetric one-dimensional box with impenetrable walls. The potential energy function for this system is given by:

$$V(x) = 0, \text{ for } -a \leq x \leq a,$$

$$V(x) = \infty, \text{ for } x < -a \text{ or } x > a.$$

Using Schrödinger wave equation calculate the energy Eigen value and the wave function for a particle in this well potential. From symmetry point of view comment why you are getting odd and even wave-functions? **(10) [BL5]**

[**Hints:** Apply the concept of 1D box for the asymmetric 1D potential box in and using that knowledge calculate it.]

Module 6: Statistical Mechanics

Statistical mechanics is a branch of physics that connects the microscopic properties of individual atoms and molecules to the macroscopic or bulk properties of materials. It provides a framework for understanding thermodynamics, phase transitions, and various other phenomena in condensed matter physics, astrophysics, and beyond.

- **Microstate:**

A microstate refers to a specific detailed microscopic configuration of a system. For a given set of particles, a microstate specifies the position and momentum of each particle.

- **Macrostate:**

A macrostate is defined by macroscopic quantities such as temperature, pressure, volume, and energy, which describe the overall state of the system without specifying the details of individual particles. Multiple microstates can correspond to the same macrostate. For example, a gas in a box with a given temperature and pressure can have countless arrangements of individual molecules (microstates) that result in the same overall conditions (macrostate).

- **Phase Space:**

Phase space is a conceptual multidimensional space in which all possible states of a system are represented. Each state is a point in this space, with dimensions corresponding to all possible values of position and momentum coordinates. For a system of N particles in three dimensions, the phase space has $6N$ dimensions, consisting of $3N$ position coordinates and $3N$ momentum coordinates. Phase space provides a complete description of a system's state. By examining trajectories in phase space, we can study the evolution of a system over time. The density of points in phase space can also be used to determine thermodynamic properties.

- **Maxwell-Boltzmann (MB) Statistics:**

Maxwell-Boltzmann statistics describe the distribution of particles in classical systems where quantum effects are negligible. It is applicable to ideal gases and assumes that the particles are distinguishable.
