Module 1 : Scalars and Vectors:

Short Questions:

1. Check whether the following sets satisfy the axioms of a real vector space.
   a) Set of all functions f(x) satisfying $\int |f(x)| dx < \infty$
   b) Set of all continuous, bounded functions defined on $0 \le x < A \quad 0 \le y < B$
   c) Set of all complex numbers of the form $a + i\,b$ where $a, b \in \mathbb{R}$, the set of real numbers.

2. Check whether the following are valid definitions of an inner product in the vector space containing the objects A and B.
   a) $A \cdot B = |AB|$ where $A, B \in \mathbb{R}$
   b) $A \cdot B = |A||B|$ where $A, B \in \mathbb{C}$, the set of complex numbers
   c) $A \cdot B = a_1 b_1 + a_2 b_2$ where $A = a_1 x + a_2 x^2 \quad B = b_1 x + b_2 x^2$

3. Evaluate whether the following set of vectors is linearly independent:
   a) (7,1) and (3,4)
   b) (1,4,2), (3,2,1),(4,0,0)
   c) (3,2,4), (1,0,1), (2,1,1) and (4,2,3)
   d) (4,3,7,-1), (2,0,1,1), (3,1,0,0), (0,0,1,0)

4. Consider a 2-body system with particle coordinates given as
   $\vec{R}_1 \equiv \{x_{1,} y_{1,} z_1\}, \vec{P}_1 \equiv \{px_{1,} py_{1,} pz_1\}$ for the first particle and
   $\vec{R}_2 \equiv \{x_{2,} y_{2,} z_2\}, \vec{P}_2 \equiv \{px_{2,} py_{2,} pz_2\}$ for the second particle, with Hamiltonian given by

   $$H(\vec{R}_{1,} \vec{P}_{1,} \vec{R}_{2,} \vec{P}_2) = px_1^2 + px_2^2 + py_1^2 + py_2^2 + pz_1^2 + pz_2^2 + x_1^2 + x_2^2 + y_1^2 + y_2^2 + z_1^2 + z_2^2$$

   Express the Hamiltonian in Center of Mass and Relative coordinates.

Long and Conceptual Questions:

1. Hilbert Space: In Quantum mechanics, we use wavefunctions to describe the state of the system. Terms like operator, eigenfunctions, eigenvalues are regularly used. The connection of Quantum Mechanics with linear algebra is explored in this part of your assignment. Consider a 1-dimensional quantum mechanical problem. The state of the system is described by a wavefunction denoted by ψ(x), and a ≤ x ≤ b. Answer the questions below with brief explanations.
   (a) First consider the set of all real functions of a single variable x defined between a and b. This set is denoted as F 1 and contains all functions of the form f (x). Show that the complete set of all such functions forms a real vector space.
   (b) Next consider those functions which are square integrable, namely those that satisfy

   $$\int_a^b |f(x)^2| dx < \infty$$

   Show that the complete set of all such functions forms a real vector space.
   (c) To convince yourself that the two sets above are not the same, give an example of a member of the first set that is not a part of the second set. You can choose the values of a and b as convenient.
   (d) Now we shall consider a different type of vector space called a complex vector space. The only difference between a complex vector space and a real vector space is that the scalars used to define the vector space can be complex numbers. Show that the set of all complex functions of a single variable that are square integrable form a complex vector space. The definition of square integrability in this case is

$$\int_a^b \overline{f(x)} f(x)\, dx < \infty$$

where $\overline{f(x)}$ is the complex conjugate of $f(x)$.

(e) What is the dimensionality of the three spaces described above ? Explain your answer.

(f) Now, we define something called a complex inner product space. In a complex inner product space, the relation between inner products (a,b) and (b,a) is given below.

$$(a,b) = \overline{(b,a)}$$

In addition the inner product of any vector with itself is nonnegative. Show that the set of complex square integrable functions forms a complex inner product space with the inner product defined as

$$(f,g) = \int_a^b \overline{f(x)}\, g(x)\, dx$$

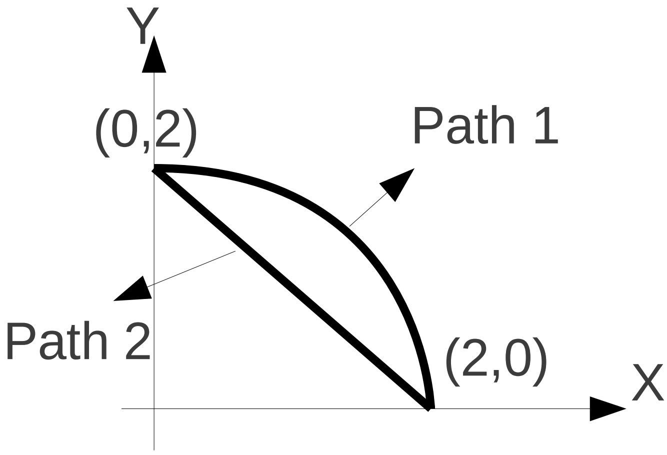
This complex inner product space is an example of a Hilbert space.

(g) Show that the Schwarz inequality and the triangle inequality hold for the Hilbert space described above.

Module 2: Vector Integration and Differentiation:

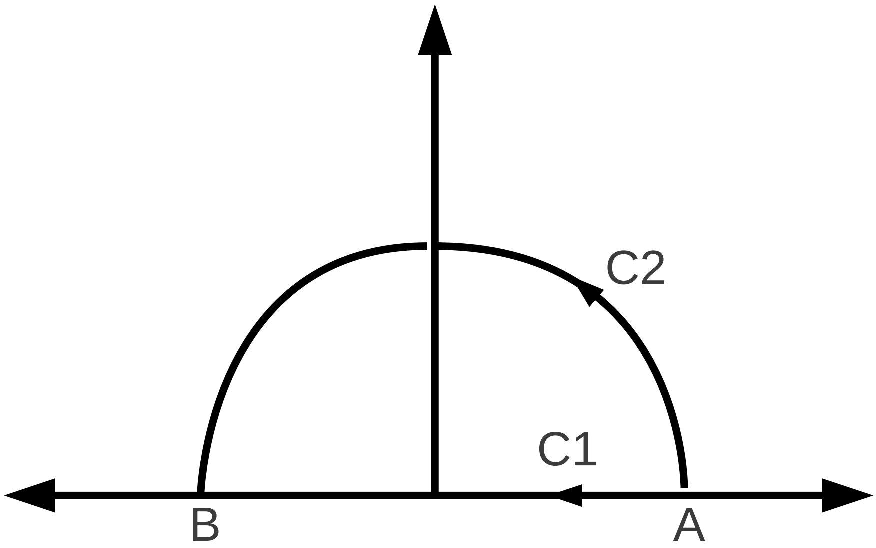
Short Questions:

1. Let $\boldsymbol{V}(x,y,z)=z(x^2+yx)\hat{x}+z(x^2+y)\hat{y}+z(x^2+y^3x)\hat{z}$
   (a) Calculate $\nabla\cdot\boldsymbol{V}$ and $\nabla\times\boldsymbol{V}$
   (b) Calculate $\oint_a^b \boldsymbol{V}\cdot d\vec{r}$ along a path specified by a parameter *t* such that at a point *a*, *t=0* and at point *b*, *t=2* π *and* $x=\cos t$ and $y=t$, $z=1$. Sketch the path of integration.
2. Starting with $\vec{F}=y\hat{x}+2x\hat{y}$, evaluate the line integral over the two paths shown below and explain whether the line integral is path dependent or not.



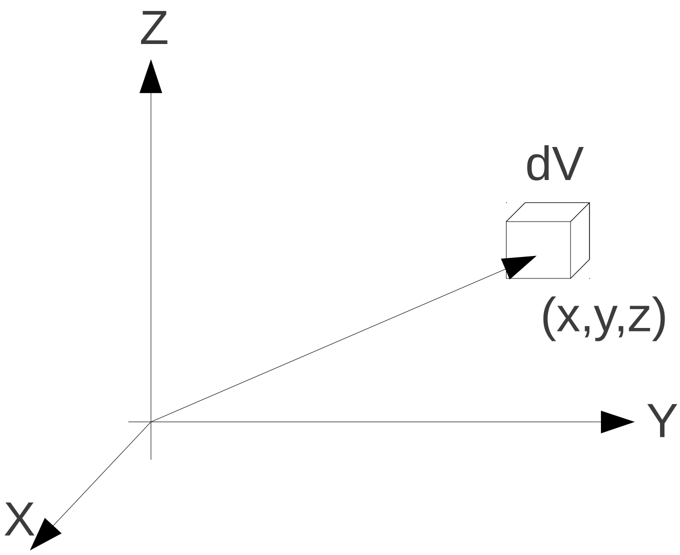
3. Calculate the work done by a force field $\vec{F}(x,y)$ in displacing a particle from *a* to *b* along the paths C1 and C2 as shown in the figure below for the two cases
   i. $\vec{F}(x,y)=(3xy-1)\hat{x}+(\frac{3}{2}x^2+4y^2)\hat{y}$
   ii. $\vec{F}(x,y)=xy\hat{x}+x^2\hat{y}$
   Comment on the path independence of the two integrals.

4. Illustrate Stokes theorem by calculating the line integral and the area integral of the curl of the following vector field $\vec{V}(x,y)=y^2\hat{i}-x^2\hat{j}$ over the region in the XY plane bounded by the circle $x^2+y^2=1$.



Long and Conceptual Questions:

1. Continuity Equation: Divergence is used in the Continuity equation in Fluid Mechanics. In fluid mechanics, we have a scalar field for the density of the fluid *ρ(x, y, z)* and a vector field for the velocity of the fluid $\vec{v}(x,y,z)=(v_x(x,y,z),v_y(x,y,z),v_z(x,y,z))$. Consider an element of the fluid at *(x, y, z)* of volume *dV = dxdydz* as shown in the figure below.



(a) Derive the net flow rate of the fluid (per unit time) in the X-direction through this volume element. Remember that the flow rate of the fluid is the amount of fluid flowing through a given volume per unit time. Write similar equations for the flow rate of the fluid through the Y and Z directions, and add the three to get a total flow rate of the fluid through the volume element *dV* .

(b) Divide both sides by *dV* to get the flow rate per unit volume through the volume element dV. Express this in terms of the divergence of the relevant quantity. The flow of the fluid through a volume causes change in the density of the fluid. Thus the flow rate per unit volume is equal to $d\rho/dt$. Equate this to the flow rate of fluid per unit volume to derive the continuity equation.

(c) Consider a fluid with a constant density and write a simplified equation.

Module 3: Matrix Algebra:

Short Questions:

1. Solve the following system of linear equations using matrix methods.
   $3x+y+z=7$
   $-2y+8z=15$
   $x+y+z=-2$
2. What is the rank of the following matrix
   $$\begin{bmatrix} 4 & 2 & -2 \\ 1 & -5 & 3 \\ 9 & 21 & -15 \end{bmatrix}$$
3. Let $A=\begin{bmatrix} 1 & 2 & -1 \\ 3 & 0 & 2 \\ 4 & 5 & 0 \end{bmatrix}$. Determine the rank of *A*. Does A^{-1} exist ? If yes, determine it.
   Find the eigenvalues and eigenvectors of *A*.
4. Let $A=\begin{bmatrix} 2 & 0 & 1-i \\ 0 & 4 & 0 \\ 1+i & 0 & 7 \end{bmatrix}$. Determine is *A* is Hermitian. Determine if *A* is Unitary.
   Calculate the eigenvalues and eigenvectors of A.
5. Calculate the rank and determinant of the matrix
   $$\begin{bmatrix} 2 & 6 & -8 & 6 \\ 8 & 2 & 4 & 0 \\ 6 & 6 & 6 & 6 \\ -2 & 2 & 7 & 4 \end{bmatrix}$$

Long and Conceptual Questions:

1. Cramer’s Rule and Gauss Elimination: In this problem, we will see how many operations are needed to calculate the determinant of a matrix using Cramer's rule and using Gauss Elimination. Let us consider the matrix

$$\left(\quad \right) \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \dots & a_{nn} \end{bmatrix}$$

First we calculate the determinant using Cramer’s rule. Recall the permutation formula for calculating the determinant

$$Det\,A=\sum_{ijkl...} \epsilon_{ijkl...}\, a_{1i}\, a_{2j}\, a_{3k} \dots$$

where *i, j, k..* are all different and *ijkl...* represents the permutation index.

(a) How many nonzero elements are in the summand above ?

(b) Calculate the total number of addition operations (substraction is also counted as an addition) used in the calculation of the determinant above. Call this number N_{add}^{Cremer} and express it in terms of n, the number of rows and columns of the A matrix.

(c) Calculate the total number of multiplication operations used in the calculation of the determinant using Cramer’s rule in terms of n.

Now we shall do the same for the determinant calculation using the method of Gauss elimination.

(a) In the first step of Gauss elimination, we convert all elements of the first column except

a_{11} to zero using $a_{ij} - \frac{a_{j1}}{a_{11}}$ for all $i \neq 1$ and all *j*. Assume that one division operation is equivalent to two multiplication operations. Calculate the total number of additions and multiplications needed in the above procedure.

(b) Repeat this procedure for the other columns until the matrix is reduced to the upper triangular form.

(c) Now the determinant of the upper triangular matrix can be calculated by a multiplying the diagonal terms. How many multiplications are involved in this process ?

(d) Now, sum up the total number of additions N_{add}^{Gauss} and multiplications N_{mult}^{Gauss} involved and show that the

$$N_{add}^{Gauss} = n(n+1)(n-1)/3 \qquad N_{mult}^{Gauss} = (n-1)(n^2+n+1)$$

Compare this number of operations required for different methods and comment on the preferred method for small and large *n*.

Module 4 :1st order ODEs

Short Questions:

Solve the following differential equations using the appropriate method:

1. $\frac{dy}{dx}=\frac{2xy}{x^2-y^2}$
2. $\frac{dy}{dx}=\frac{y-x^2}{x}$ using the substitution $u=\frac{x}{y}$
3. $\frac{dy}{dx}=e^{-3x}+\cos(4x)$ with the boundary condition y=3 when x=0.
4. $\frac{dy}{dx}=2y+\cos(4x)$
5. $\frac{dy}{dx}=\frac{4x^3+2xy+1}{4y^3-x^2-7}$
6. $\frac{dy}{dx}=\frac{3y^2\sin(x)+2xy\cos(y)}{x^2y\sin(y)+x^2\cos(y)}$

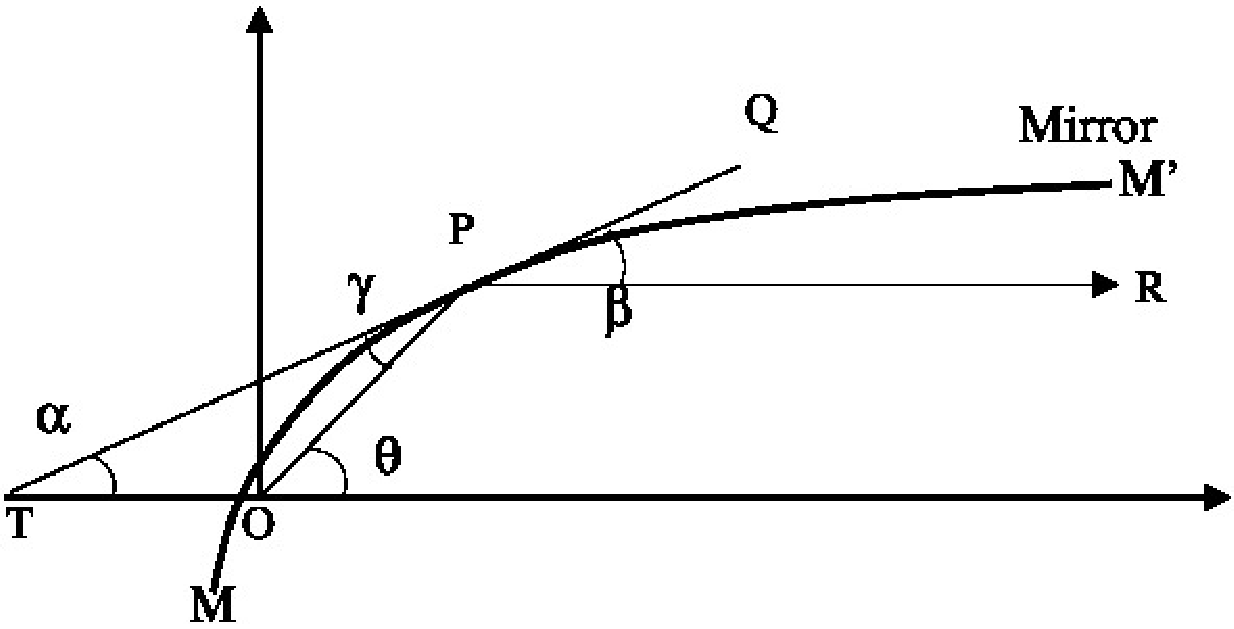
Long and Conceptual Questions:

1. Coupled Unimolecular Reactions: Consider the set of elementary unimolecular reactions given by

$$A \xrightarrow{k_1} B \underset{k_{-2}}{\overset{k_2}{\Leftrightarrow}} C \xrightarrow{k_3} D$$

(a) Write the rate equations for these reactions.
(b) Consider a four component vector denoted by $\vec{y}$ given by *([A], [B], [C], [D])* where the square brackets denote the concentration of the species. Write a differential equation for $d\vec{y}/dt$.
(c) Consider a trial function of the form $\vec{y}=\vec{y}_0 e^{\lambda t}$. Substitute in the equation and identify what $\vec{y}_0$ and λ are related to.
(d) Solve the equations for $k_1 = 1, k_2 = 2, k_{-2} = 1, k_3 = 2$ with initial conditions *[A](0) = A* and *[B](0) = [C](0) = [D](0) = 0.*

2. Parabolic Mirror: In this exercise, we will derive the equation of a curve such that a mirror of that shape always reflects light from a point source at the origin along the positive x-direction. In the figure the thick curve represents the mirror. Light from the origin strikes the mirror at P and is reflected towards R parallel to the X-axis. PQ represents the local tangent to the curve at P and intersects the X-axis at T. Our goal is to find the equation of the curve. Note that light striking the curve anywhere is always reflected along the positive X-axis. The angles α, β, θ and γ are defined as shown in the figure .



(a) What are the relations between the angles α, β, θ and γ ?

(b) If the curve is described by a function *y(x)*, express the angles α and θ in terms of *y, x* and the appropriate derivatives.

(c) Use the relation between θ and θ in part (a) to derive a relationship between *y, x* and $y = dy/dx$.

(d) Express *y* in terms of *x* and *y*.

(e) Solve the resulting first order differential equations by rearranging the terms in the form of an exact differential.

Module 5: 2nd order differential equations

Short Questions:

1. Consider the following equation

$$\frac{d^2y}{dx^2}+6\frac{dy}{dx}+25\,y=a^2\sin(kx)$$

where k is a positive real number. What is the general solution of this equation ?

2. Find a general solution of the following differential equation $x^2y''-2xy'+2y=x\ln x$ by first solving the homogeneous differential equation and using the method of linear variations to identify the general solution of the inhomogeneous equation.

Long and Conceptual Questions:

1. The Wave Equation:

The equation of a wave in one dimension is given by $\frac{\partial^2 y(x,t)}{\partial x^2}=\frac{1}{v^2}\frac{\partial^2 y(x,t)}{\partial t^2}$ where v is a constant equal to the velocity of the wave and y(x,t) is the amplitude of the wave at position x and time t. This is a partial differential equation but it can be solved by a technique known as separation of variables.

(a) Assume that $y(x,t)=X(x)T(t)$ where X(x) is a function of x and T(t) is a function of t. Is this assumption always true ? If not, can you think of a counter example ?

(b) Substitute the form of y(x,t) above in the wave equation. Divide both sides by X(x)T(t). You should get an equality involving X on the left hand side and T on the right hand side.

(c) Explain why both terms in the equality above should be equal to a constant. Assume that this constant is negative (to get stable solutions).

(d) Write two separate ordinary differential equations for X(x) and T(t). Solve each of them and write the total solution.

(e) In 2-dimensions, the wave equation is written as $\nabla^2 y(x,y,t)=\frac{1}{v^2}\frac{\partial^2 y(x,y,t)}{\partial t^2}$

Write this equation in polar coordinates (r,θ).

(f) Now, write y(r,θ,t) = R(r)Θ(θ)T(t). Substitute in the above equation and try to write separate equations.

(g) The boundary condition is of the form *y(A*,θ,t)=0 where A is some distance. This corresponds to a drum of radius A and the wave equation describes the vibrations of the drum. Write down the separated equations when the amplitude y is independent of θ. Assume, like in part(c), that the constant is negative and equal to $-l^2$. Solve the differential equation for T(t).

(h) Set $q=lr$ in the differential equation for R(r) and obtain a differential equation for q. This equation corresponds to a special case of a very well known equation in engineering called Bessel's differential equation.

(i) This equation is not like the typical second order differential equation with polynomial coefficients, because it has coefficients with negative powers of x. To solve this equation, we write $R(q)=\sum_{i=0}^{\infty} c_m q^{m+p}$ where p is a real or complex number chosen so that $c_0\neq 0$. This is a small modification to the power series method and is called the Frobenius method.

Substitute this form of R(q) into the differential equation to obtain the the equation involving sums of terms like you do in any power series solution.

(j) Equate the coefficients of q^p in the equation. What are the allowed values of p ?

(k) Substitute the allowed value of p into the equation in part (i). Now, follow the procedure used in the power series method to write relations between coefficients and the recursion relation.

(l) Write all the coefficients in terms of c_0 .

(m) Since c_0 can be chosen arbitrarily, we choose $c_0=1$. Calculate all the other coefficients. The solution R(q) corresponds to the Bessel Function of the first kind of order 0, commonly denoted as $J_0(q)$

(n) To satisfy the boundary condition, we need to know the roots of the Bessel function i.e. what are the values of α such that $J_0(\alpha)=0$. These are numerically calculated and it is observed that the Bessel function has infinite roots. Thus there are infinitely many functions that can satisfy the boundary condition and the differential equation, and these correspond to the different normal modes. The first three roots of $J_0(\alpha)$ occur at $\alpha=2.4048, \alpha=5.5201,$ and $\alpha=8.6537$. Write the solutions for R(r) corresponding to these roots in terms of Bessel functions of arguments involving r and A.

Module 6: Integral Transforms:

Short Questions:

1. Show that the Fourier transform of a Gaussian function in one-dimensions is also a Gaussian function and derive the relation between the standard deviations of the two Gaussians.

Long and Conceptual Questions:

1. Consider the polynomials $P_n(x)$ where

$$P_0(x)=1 \quad \text{and} \quad P_n(x)=\frac{e^x}{n!}\frac{d^n}{dx^n}x^n e^{-x} \quad \text{for n=1,2,3...}$$

(a) Calculate the polynomials for n=1,2 and 3.

(b) What is the value of $P_n(0)$ for arbitrary n. Explain your answer.

(c) Write a representation for $P_n(x)$ in the form of series. How many terms are present in the series ?

(d) $G(x,z)=\frac{e^{-xz/(1-z)}}{1-z}$ is the generating function for the polynomials $P_n(x)$. Thus, $|\frac{\partial^n G(x,z)}{\partial z^n}|_{z=0}$ is related to the polynomial $P_n(x)$. By calculating these quantities for the first few polynomials, guess the exact relationship between the generating function and the polynomials.

(e) Starting with $G(x,z)=\frac{e^{-xz/(1-z)}}{1-z}$, differentiate both sides w.r.t. z. Eliminate $e^{-xz/(1-z)}$ to get a partial differential equation for G(x,z) involving derivative w.r.t. z. Rearrange terms and substitute the relation that you derived in part (d) so you get a recursion relation involving $P_{n+1}(x), P_n(x)$ and $P_{n-1}(x)$

(f) Starting with $G(x,z)=\frac{e^{-xz/(1-z)}}{1-z}$, differentiate both sides w.r.t. x. Eliminate $e^{-xz/(1-z)}$ to get a partial differential equation for G(x,z), this time involving derivative w.r.t. x. Rearrange terms and substitute the relation that you derived in part (d) so you get another recursion relation involving $P'_{n-1}(x), P'_n(x)$ and $P_{n-1}(x)$.

(g) Combine the Partial Differential equations you derived for G(x,z) in part(e) and part(f) to derive the following relation

$$x\frac{\partial G}{\partial x}=z\frac{\partial G}{\partial z}-z\frac{\partial (zG)}{\partial z}$$

(h) Substitute the relation you derived in part (d) to get a third recursion relation, this time involving $P'_n(x), P_n(x)$ and $P_{n-1}(x)$.

(i) Use the three recursion relations to derive a second order differential equation for $y=P_n(x)$

(j) Is the equation in part (h) of the form of the Sturm-Liouville problem ? If not, then multiply the equation by a factor u(x) so that it is in the form of the Sturm-Liouville problem. By comparing the coefficients of y'' and y', you should be able to derive a simple differential equation for u(x) and solve for u(x). By choosing the limits as 0 and ∞, show that this is a Sturm-Liouville Problem.

(k) Verify that the polynomials $P_n(x)$ are orthogonal w.r.t. the weight function u(x) that you derived in part (i) explicitly by showing that the appropriate integral equals zero.

2. Find the general solution for y(x) for the equation below where k is a real number

$$y'' + k^2 y = 1$$

(a) Evaluate whether the differential equation can be expressed in the form of a Sturm-Liouville differential equation.

(b) Use $y(\pi) = y(-\pi)$ and $y'(\pi) = y'(-\pi)$. Find the appropriate solution in this case and write the Orthogonality relation (if any) predicted by this equation.

3. Principle of superposition: The principle of superposition is one of the fundamental postulates of Quantum Mechanics. It states that a general state of the system can be represented as a linear combination of eigenstates of ANY linear Hermitian operator (that corresponds to some physical observable). In order to use this, we have to pick eigenstates that form a basis; in other words they should be linearly independent. Note that the general state need not be an eigenstate of that observable. For this purpose, it is essential that the eigenstates of operators should form a basis. Let us explore this principle in some practical applications. We will assume 1-D position space, so all states are functions of a single variable *x*. We will start with the variable linear momentum *p*.

(a) If the expression for an operator consists of a differential, then the eigenvalue equation is a homogenoeous differential equation. Justify the above expression and illustrate by considering examples of 3 such operators.

(b) What are the eigenfunctions of the linear momentum corresponding to a real eigenvalue p ? What is the number of eigenfunctions in the basis ?

(c) If the particle is in a state given by $\psi(x) = a\sin(kx)$, write this state as a linear superposition of momentum eigenstates.

(d) Now write the state $\psi(x) = a\sin(kx) + b\sin^3(kx)$ as a linear combination of eigenstates of linear momentum.

(e) If $\psi_1(x)$ and $\psi_2(x)$ are eigenfunctions of momentum, is $c_1\psi_1(x) + c_2\psi_2(x)$ also an eigenfunction of momentum ? Justify your answer using your knowledge of homogeneous differential equations.

(f) Write e^{-ax} as a linear superposition of eigenstates of the momentum operator.

(g) What is the general form for the eigenfunctions of $p^2 + \hat{p}$?

4. Consider the partial differential equation given by

$$\frac{\partial^4 y}{\partial x^4} + \frac{1}{a^2}\frac{\partial^2 y}{\partial t^2} = 0$$

subject to initial conditions at *t=0* given by

$$y(x) = f(x) \quad \text{and} \quad \frac{\partial y}{\partial t} = a\frac{\partial^2 g(x)}{\partial x^2}$$

where *f(x)* and *g(x)* are well-behaved functions and *a* is a real number.

(a) Express the PDE in FT domain by transforming *x* to *k*. The resulting equation is a ODE in terms of time for $\tilde{y}(k,t)$

(b) Solve the resulting ODE to obtain $\tilde{y}(k,t)$ subject to the initial conditions.

(c) Invert the result to obtain the solution for the *y(x, t)*. The solution will be in the form of a convolution involving *f (x)* and *g(x)*.

(d) Consider $f(x) = \alpha e^{-x^2/4x_0^2}$ and *g(x) =0* and derive the solution.

Module 7: Group Theory Basics:

Short Questions:

1. What is the difference between a subgroup and a class of a group ? Do all elements of a subgroup belong to the same class ? Do all elements of a class form a subgroup ? Explain with examples.
2. Identify the various symmetry operations of the ammonia molecule. Construct the group multiplication table and identify the classes.
3. Identify the symmetry operations in staggered and eclipsed ethane molecule.

Long and Conceptual Questions:

1. Lagrange's theorem implies that the order of a subgroup must divide the order of a group. The proof of this theorem is a standard exercise in abstract algebra. In this problem, we use similar techniques to prove that number of elements in a class of a group must divide the order of a group.

(a) Consider a group G consisting of g elements $\{A_1,A_2,A_{3......}A_g\}$ and a suitably defined binary operation. Now let B be a class in G consisting of c elements $\{A_1,A_2,A_{3......}A_c\}$ and the same binary operation. Write down clearly the property which the elements of B must satisfy.

(b) Following the method of proof that the order of a subgroup divides order of the group, first consider the trivial cases when B contains one single element and when B is the entire group and show that the theorem holds for these cases.

(c) If B contains just one element, what can you say about the commutation properties of that element with other elements in G ?

(d) Let Z(G) be the set of elements of G which commute with all elements of G. Show that Z(G) is a subgroup of G. Z(G) is called the *center* of G.

(e) Since Z(G) is a subgroup of G, order of Z(G) divides order of G. Now consider an element A_i contained in B. The set of elements in G that commute with A_i is called the *centralizer* of A_i in G and is denoted by $C_G(A_i)$. Show that $C_G(A_i)$ is a subgroup of G.

(f) Now consider an element g of G and an element A_i of B. Now consider the operation of conjugation of A_i or $g^{-1}A_ig$ where g is an element of G. What happens when $g \in C_G(A_i)$?

(g) Now consider conjugation of A_i by ALL members of G. This gives the set B. Moreover, you can show that when you examine all the terms of the form $g^{-1}A_ig$, you get each element of B an integer number of times and that integer is equal to the order of the $C_G(A_i)$.

(h) Finally show that the order of a class is a factor of the order of a group and express the factor in terms of order of $C_G(A_i)$.

Module 8: Symmetry groups of molecules:

Short Questions:

1. Draw a 3-D molecule (need not be a real molecule) that has an S8 axis but no C8 axis and no σ_h . Explain the axis clearly.
2. Identify the symmetry elements and classes and symmetry group of the following molecules:
   (a) $CH\,Cl_3$ (b) Staggered and Eclipsed Ethane (c) Ammonia
   (d) Trans $[Co\,Cl_2(NH_3)_4]^+$ complex
3. For each symmetry operation, identify the equivalent atoms in Staggered Ethane.
4. For water, identify the equivalent symmetry operations.

Long and Conceptual Questions:

For each of the following molecules, write down all the symmetry operations and the group multiplication table. Identify the classes of symmetry operations and identify the groups they belong to:

1. H_2S 2. CH_2ClBr 3. HCHO

Module 9: Group Character Table:

Short Questions:

1. Matrix Representation of symmetry operations:
 (a) What is the general equation of a line in 3-D ? There are many forms of this but make sure you use one of the general forms.
 (b) What is the general equation of a line passing through the origin ?
 (c) Using the above line as a symmetry element, find the 3X3 matrix representation of a C_n rotation about this axis.
 (d) What is the general equation of a plane in 3D passing through the origin ?
 (e) Calculate the 3X3 matrix representation for reflection about this plane.
 (f) Is the product of two rotations another rotation ? Justify your answer.
 (g) Is the product of two reflections another reflection ? Justify your answer.

2. Consider the group C_{3v}. What are the 3X3 matrix representations of all the operations of this group ? Show that this is a reducible representation by block factorization of the matrix representations. What are the dimensions of the irreducible representations thus obtained ? What are the characters of the various classes in these irreducible represntations ?

3. Consider the group D_{3h}. Use the character table of this group and the Great Orthogonality Theorem to express the representation Γ in terms of irreducible representations of the group. The characters of the classes in the representation Γ are:
$\chi(E)=8 \;, \chi(2C_3)=2 \;, \chi(3C_2)=2 \;, \chi(\sigma_h)=0 \;, \chi(2S_3)=6 \;, \chi(3\sigma_v)=2$

Long and Conceptual Questions:

1. Starting from the multiplication table for D_{3h}, identify the various classes in this group. Using these classes, we can construct the character table of the group as follows:
   (a) First write down the matrix elements (3X3) for all the 12 operations of the group. Clearly specify your coordinate system for this problem before writing the matrix elements. Write the multiplication table for this group.
   (b) Write down the number and dimensionality of the irreducible representations of this group.
   (c) Starting with the characters of E, derive the characters of the irreducible representations. Show all the steps involved in this process and describe clearly the logic that you have used.
   (d) Is the representation you derived in part (a) irreducible ? Why or why not ? If it is reducible, then represent the characters of the reducible representation in terms of characters of irreducible representations.
   (e) Starting with the matrix representation (3X3) of the elements of the group, find by observation, the similarity transformation that converts this matrix into block diagonal forms where each of the blocks corresponds to an irreducible representation. You can use the multiplication table for this purpose. While this exercise seems to be extremely unwieldy since you have so many operations, you can actually use fairly simple logic to come up with the appropriate transformation.

Module 10: Group Theory and Quantum Mechanics:

Short Questions:

1. Consider the effect of the operations of C_{2v} on the two OH bonds in water and predict how many independent stretching vibrations are present in water.
2. In the above question, use the projection operator to find out to which irreducible representations the two vibrations above belong to.
3. Use the direct product rules to find out how the d_{xy},d_{xz} and d_{yz} orbitals transform under each of the symmetry operations in the group D_{2d}. Assume that the orbitals are located on the central atom.

Long and Conceptual Questions:

1. Consider the three-dimensional representation formed by the three NH stretches in NH_3 molecule. What are the characters of the classes in this representation ? Express this representation in terms of irreducible representations. Use the Projection operator method to find the independent stretching vibration modes of NH_3 molecule. How many of these independent vibrations are degenerate ?
2. Cyclobutadiene belongs to point group D_{2h}. Consider the 4 p_z orbitals on the 4 carbon atoms of cyclobutadiene and construct a 4-dimensional reducible representation. Use the Character table of the group to express this reducible representation in terms of irreducible representations of the group. Next, construct a symmetry adapted linear combinations of the 4 p_z orbitals by projecting the SALCs obtained from any one orbital onto the irreducible representations.

Module 11: Data Analysis:

Short Questions:

1. The table below gives the values of the rate constant of a first order reaction in s^{-1} for 10 different measurements.

No	1	2	3	4	5	6	7	8	9	10
Rate	4.25	4.10	4.33	4.21	4.45	4.30	4.17	4.21	4.12	4.37

Use this table to calculate the average, standard deviation and error estimate of the reported average. How would you report such a reading in terms of significant figures ?