Imperial College London

NOTES

IMPERIAL COLLEGE LONDON

DEPARTMENT OF PHYSICS

Mathematical Methods for Physicists

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1 Vector Spaces and Tensors

1.1 vector spaces

1.1.1 Definition of a Vector Space

Definition. A real (complex) vector space is a set \mathbb{V} - whose elements are called vectors - together with two operations called addition (+) and scalar multiplication such that

- 1. \mathbb{V} is closed under **addition**: $\forall \underline{u}, \underline{v} \in \mathbb{V} \Rightarrow \underline{u} + \underline{v} \in \mathbb{V}$.
- 2. \mathbb{V} is closed under scalar multiplication: $\forall \underline{u} \in \mathbb{V}$ and \forall scalar $\lambda \Rightarrow \lambda \underline{u} \in \mathbb{V}$.
- 3. There exists a null or zero vector $\underline{0}$ such that $\underline{u} + \underline{0} = \underline{u}$.
- 4. Each vector \underline{u} has a corresponding negative vector $-\boldsymbol{v}$ such that: $\underline{u} + (-\underline{v}) = 0$.
- 5. The addition operation satisfies: $\underline{u} + \underline{v} = \underline{v} + \underline{u}$ and $(\underline{u} + \underline{v}) + \underline{w} = \underline{u} + (\underline{v} + \underline{w})$.
- 6. Scalar multiplication satisfies: $a(\underline{u} + \underline{v}) = a\underline{u} + a\underline{v}, \ a(b\underline{u}) = (ab)\underline{u}$

Example. 3 component real column vectors

$$\mathbb{R}^3 = \left\{ \begin{pmatrix} a \\ b \\ c \end{pmatrix} \middle| a, b, c \in \mathbb{R} \right\}$$

2 component complex vectors

$$\mathbb{C}^2 = \left\{ \begin{pmatrix} x \\ y \end{pmatrix} \middle| x, y \in \mathbb{C} \right\}$$

1.1.2 Linear Independence

Definition. A set of n non-zero vectors $\{u_1, u_2, \dots, u_n\}$ in a vector space is linearly independent if

$$\sum_{i=1}^{n} a_i u_i = 0 \quad \Rightarrow \quad a_i = 0 \quad \forall i$$

Otherwise we say $\{u_1, u_2, \cdots, u_n\}$ is linearly dependent.

Let N be the maximum number of linearly independent vectors in \mathbb{V} , then N is the dimension of \mathbb{V} .

Definition. A subspace, \mathbb{W} , of a vector space \mathbb{V} is a subset of \mathbb{V} that is itself a vector space.

1.1.3 Basis Vectors

Any set of n linearly independent vectors $\{u_i\}$ in an n-dimension vector space \mathbb{V} is a *basis* for \mathbb{V} . Any vector v in \mathbb{V} can be represented as a linear combination of the basis vectors

$$v = \sum_{i=1}^{n} a_i u_i$$

1.1.4 Inner Product

Definition. An inner product on a **real vector space** \mathbb{V} , is a **real** number $\langle \underline{u}, \underline{v} \rangle$ for every pair of vectors \underline{u} and \underline{v} . The inner product has the following properties

- 1. $\langle \underline{u}, \underline{v} \rangle = \langle \underline{v}, \underline{u} \rangle$
- 2. $\langle \underline{u}, a\underline{v}_1 + b\underline{v}_2 \rangle = a\langle \underline{u}, \underline{v}_1 \rangle + b\langle \underline{u}, \underline{v}_2 \rangle$
- 3. $\langle v, v \rangle \geq 0$
- 4. Define $\|\underline{v}\| = \sqrt{\langle \underline{v}, \underline{v} \rangle}$. Then $\|\underline{v}\| = \underline{0} \implies \underline{v} = \underline{0}$

Definition. An inner product on a **complex space** \mathbb{V} , is a **real** number $\langle u, v \rangle$ for every ordered pair of vectors u and v. The inner product has the following properties

- 1. $\langle \underline{u}, \underline{v} \rangle = \langle \underline{v}, \underline{u} \rangle^*$
- $\begin{array}{l} \textbf{2.} \ \, \langle \underline{u}, a\underline{v}_1 + b\underline{v}_2 \rangle = a \langle \underline{u}, \underline{v}_1 \rangle + b \langle \underline{u}, \underline{v}_2 \rangle \\ \, \langle a\underline{u}_1 + b\underline{u}_2, v \rangle = a^* \langle \underline{v}, \underline{u}_1 \rangle^* + b^* \langle \underline{v}, \underline{u}_2 \rangle^* = a^* \langle \underline{u}_1, \underline{v} \rangle + b^* \langle \underline{u}_2, \underline{v} \rangle \\ \end{array}$
- 3. $\langle v, v \rangle > 0$
- 4. Define $\|\underline{v}\| = \sqrt{\langle \underline{v}, \underline{v} \rangle}$. Then $\|\underline{v}\| = 0 \implies \underline{v} = \underline{0}$

Example.

$$\mathbb{R}^{3} = \left\langle \begin{pmatrix} a \\ b \\ c \end{pmatrix}, \begin{pmatrix} d \\ e \\ f \end{pmatrix} \right\rangle = ad + be + cf, \qquad \mathbb{C}^{2} = \left\langle \begin{pmatrix} a \\ b \end{pmatrix}, \begin{pmatrix} c \\ d \end{pmatrix} \right\rangle = a^{*}c + b^{*}d$$

1.1.5 Orthogonality

Two vectors are said to be **orthogonal** if their inner product is zero, i.e.

$$\langle \underline{u}, \underline{v} \rangle = 0 \tag{1}$$

A set of vectors $\{\underline{e}_1, \cdots, \underline{e}_n\}$ is **orthonormal** if

$$\langle \underline{e}_i, \underline{e}_j \rangle = \delta_{ij} = \begin{cases} 0, & i \neq j \\ 1, & i = j \end{cases}$$
 (2)

where δ_{ij} is named as Kronecker delta.

1.2 Matrices

A $m \times n$ matrix is an array of numbers with with m rows and n columns.

1.2.1 Summation Convention

The expression for the elements of C = AB is

$$C_{ij} = \sum_{k} A_{ik} B_{kj} \tag{3}$$

and this may be written as

$$C_{ij} = A_{ik}B_{kj} \tag{4}$$

where it is implicitly assumed that there is a summation over the repeated index k. This shorthand is known as the *Einstein summation convention*. In this expression, k is called a *dummy index*, and i and j are called as *free indices*.

There are three basic rules to index notation:

- 1. In any one term of an expression, indexes may appear only once, twice or not at all.
- 2. A index that appears only once on one side of an expression must also appear once on the other side. It is called a *free index*.
- 3. A index that appears twice is summed over. It is called a *dummy index*.

1.2.2 Recall Special Square Matrices

· Unit matrix.

$$\mathbb{I} = \begin{pmatrix}
1 & 0 & 0 & \cdots \\
0 & 1 & 0 & \cdots \\
0 & 0 & 1 & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix}$$
(5)

- Unitary matrix. U is unitary if $UU^{\dagger} = U^{\dagger}U = \mathbb{I}$
- Symmetric and anti-symmetric matrices. S is symmetric, if $S^T = S$ or, alternatively, $S_{ij} = S_{ji}$. A is anti-symmetric if $A^T = -A$ or, alternatively, $A_{ij} = -A_{ji}$.
- Hermitian and anti-Hermitian matrices. These may be thought of as the complex generalisations of symmetric and anti-symmetric matrices. H is Hermitian if $H^{\dagger} = H$ or, alternatively, $H_{ij} = H_{ji}^*$. A is anti-Hermitian if $A^{\dagger} = -A$ or, alternatively, $A_{ij} = -A_{ji}^*$.
- Orthogonal matrix. R is orthogonal, if it satisfies

$$R^T R = R R^T = \mathbb{I} \quad \Leftrightarrow \quad R^T = R^{-1} \tag{6}$$

1.2.3 Levi-Civita Symbol (Alternating Tensor or Epsilon Tensor)

The Levi-Civita symbol has three indices, each of which can take value 1,2 or 3 and is defined as

$$\varepsilon_{ijk} = \begin{cases} 1, & (i, j, k) = (1, 2, 3), (2, 3, 1), (3, 1, 2) \\ -1, & (i, j, k) = (3, 2, 1), (2, 1, 3), (1, 3, 2) \\ 0, & \text{otherwise} \end{cases}$$
 (7)

The alternating tensor can be used to write 3-d Euclidean vector (cross) products in index notation:

$$c = a \times b \quad \Leftrightarrow \quad c_i = \varepsilon_{ijk} a_j b_k$$
 (8)

A useful identity involving the contraction of two alternating tensors is

$$\varepsilon_{ijk}\varepsilon_{klm} = \delta_{il}\delta_{im} - \delta_{im}\delta_{il} \tag{9}$$

Example. we can use it to prove the vector identity $\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = (\mathbf{a} \cdot \mathbf{c})\mathbf{b} - (\mathbf{a} \cdot \mathbf{b})\mathbf{c}$.

$$[\boldsymbol{a} \times (\boldsymbol{b} \times \boldsymbol{c})]_{i} = \varepsilon_{ijk} a_{j} (\boldsymbol{b} \times \boldsymbol{c})_{k}$$

$$= \varepsilon_{ijk} a_{j} \varepsilon_{klm} b_{l} c_{m}$$

$$= (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) a_{j} b_{l} c_{m}$$

$$= (a_{j} c_{j}) b_{i} - (a_{j} b_{j}) c_{i}$$

$$= (\boldsymbol{a} \cdot \boldsymbol{c}) [\boldsymbol{b}]_{i} - (\boldsymbol{a} \cdot \boldsymbol{b}) [\boldsymbol{c}]_{i}$$
(10)

1.2.4 Eigenvalues, Eigenvectors and Diagonalization

An eigenvalue equation takes the form

$$A_{ij}x_j = \lambda x_i \tag{11}$$

where A_{ij} are the components of an $n \times n$ matrix, and x is an eigenvector with corresponding eigenvalue λ .

Form the $n \times n$ matrix M whose n columns are the vectors $\{e^{(1)}, ... e^{(n)}\}$. Then M is an orthogonal matrix and

$$M^{\dagger}AM = \begin{pmatrix} \lambda_1 & 0 \\ & \ddots & \\ 0 & \lambda_n \end{pmatrix} \tag{12}$$

1.3 Scalars, Vectors and Tensors in 3d Space

- Scalar quantities have magnitude and are independent of the any direction.
- **Vector** quantities have magnitude and direction.
- Rank-two tensor quantities are an extension of the concept of a vector, and each has two indices.

$$J_i = \sigma_{ij} E_i \tag{13}$$

1.4 Transformations under Rotations

1.4.1 Transformation of Vectors

The two sets of components of x are related by an orthonal matrix L and det(L) = 1

$$x_i' = L_{ij}x_i \tag{14}$$

Set of all such matrices form SO(3) group.

1.4.2 Transformation of Rank-Two Tensors

A rank-two tensor transforms as

$$T'_{ij}(x') = L_{ip}L_{jq}T_{pq}(x) \quad \Leftrightarrow \quad T' = LTL^T$$
(15)

For higher rank tensor,

$$T'_{ijk\cdots}(x') = L_{ip}L_{jq}L_{kr}\cdots T_{pqr\cdots}(x)$$
(16)

1.5 Tensor Calculus

1.5.1 The Gradient Operator

$$\nabla = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}\right) \tag{17}$$

The definitions of grad, div and curl in Cartesian coordinates may be expressed using index notation:

$$[\nabla \phi]_i = \partial_i \phi \tag{18}$$

$$\nabla \cdot \mathbf{F} = \partial_i F_i \tag{19}$$

$$(\nabla \times \mathbf{F})_i = \varepsilon_{ijk} \partial_j F_k \tag{20}$$

where we have used the convenient shorthand $\partial_i = \frac{\partial}{\partial x_i}$.

2 Green Functions

2.1 Introduction

Green functions are an invaluable tool for the solution of inhomogeneous differential equations. Here we consider the second-order linear *ordinary differential equation* (ODE) with some boundary conditions. \mathcal{L} is a linear second order differential operator, and

$$\mathcal{L}_x[y(x)] = \left[\frac{\mathrm{d}}{\mathrm{d}x^2} + p(x) \frac{\mathrm{d}}{\mathrm{d}x} + q(x) \right] y(x) = f(x)$$
 (21)

The range of the parameter x is $x \in [\alpha, \beta]$ where α might be finite or $-\infty$ and β might be finite or $+\infty$. f(x) is a known function. If f(x) = 0, the ordinary is **homogeneous**; while when $f(x) \neq 0$, the equation is **inhomogeneous**.

Suppose that we know $y_1(x), y_2(x)$ are solutions of $\mathcal{L}_x[y(x)] = 0$, and they are linearly independent.

2.2 Variation of Parameters

From the assumptions above, we know that

$$y(x) = ay_1(x) + by_2(x) (22)$$

is a set of $\mathcal{L}_x[y(x)] = 0$ for any constant a and b, and

$$y(x) = ay_1(x) + by_2(x) + y_0(x)$$
(23)

is a solution of $\mathcal{L}_x[y(x)] = f(x)$. y_0 is called particular integral, and is any solution of $\mathcal{L}_x[y(x)] = f(x)$.

Imposing the boundary conditions of a particular problem will result in equations for the numbers a and b in the general solution. These equations can be solved for a and b. Two boundary conditions will give two equations for the two unknown constants a and b.

We assume that the particular integral of ode is given by

$$y_0(x) = u(x)y_1(x) + v(x)y_2(x)$$
(24)

and the differential

$$y_0' = u'y_1 + uy_1' + v'y_2 + vy_2'$$
(25)

$$y_0'' = u''y_1 + 2u'y_1' + uy_1'' + v''y_2 + 2v'y_2' + vy_2''$$
(26)

Substituting these expressions into the eqn.(21)

$$\mathcal{L}_{x}[y_{0}(x)] = u''y_{1} + 2u'y'_{1} + uy''_{1} + v''y_{2} + 2v'y'_{2} + vy''_{2} + p(u'y_{1} + uy'_{1} + v'y_{2} + vy'_{2}) + q(uy_{1} + vy_{2}) = u(y''_{1} + py'_{1} + qy_{1}) + v(y''_{2} + py'_{2} + qy_{2}) + u''y_{1} + 2u'y'_{1} + v''y_{2} + 2v'y'_{2} + p(u'y_{1} + v'y_{2}) = u''y_{1} + 2u'y'_{1} + v''y_{2} + 2v'y'_{2} + p(u'y_{1} + v'y_{2})$$
(27)

Therefore, we will vary these parameters subject to the constraint

$$u'y_1 + v'y_2 = 0 (28)$$

and

$$u''y_1 + u'y_1' + v''y_2 + v'y_2' = 0 (29)$$

Substituting these expressions into the differential equation (21), after some rearrangement, gives

$$u'y_1' + v'y_2' = f$$
 (30)

So we have

$$\begin{cases} u'y_1' + v'y_2' = f \\ u'y_1 + v'y_2 = 0 \end{cases} \Rightarrow \begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix} \begin{pmatrix} u' \\ v' \end{pmatrix} = M \begin{pmatrix} u' \\ v' \end{pmatrix} = \begin{pmatrix} 0 \\ f \end{pmatrix}$$
 (31)

then

$$\begin{pmatrix} u' \\ v' \end{pmatrix} = M^{-1} \begin{pmatrix} 0 \\ f \end{pmatrix} = \frac{1}{W(x)} \begin{pmatrix} y_2' & -y_2 \\ -y_1' & y_1' \end{pmatrix} \begin{pmatrix} 0 \\ f \end{pmatrix}$$
(32)

where W(x) is the Wronskian, and

$$W(x) = \det(M) = y_1 y_2' - y_2 y_1'$$
(33)

So the solutions are

$$u'(x) = -\frac{y_2(x)f(x)}{W(x)}, \qquad v'(x) = \frac{y_1(x)f(x)}{W(x)}$$
(34)

2.2.1 Homogeneous Initial Conditions

The boundary conditions $y(\alpha) = y'(\alpha) = 0$ are called *homogeneous initial conditions*. Integrating eqn. (34) gives

$$u(x) = -\int_{\alpha}^{x} d\tilde{x} \frac{y_2(\tilde{x})f(\tilde{x})}{W(\tilde{x})}, \qquad v(x) = \int_{\alpha}^{x} d\tilde{x} \frac{y_1(\tilde{x})f(\tilde{x})}{W(\tilde{x})}$$
(35)

then

$$y_0(x) = u(x)y_1(x) + v(x)y_2(x) = \int_0^x d\tilde{x} \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x})$$
(36)

satisfies $y_0(\alpha) = y_0'(\alpha) = 0$. So $y = y_0$ is a solution of the ODE with boundary conditions $y(\alpha) = y'(\alpha) = 0$.

$$y(x) = \int_{\alpha}^{x} d\tilde{x} \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) + \int_{x}^{\beta} d\tilde{x} \cdot 0$$

$$= \int_{\alpha}^{\beta} G(x, \tilde{x}) f(\tilde{x}) d\tilde{x}$$
(37)

where we have defined the Green Function

$$G(x, \tilde{x}) = \begin{cases} 0, & x < \tilde{x} \\ \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})}, & x > \tilde{x} \end{cases}$$
(38)

Figure 1: The range of variable x in the problem is $x \in [\alpha, \beta]$.

2.2.2 Inhomogeneous Initial Conditions

Consider more general initial conditions of the form $y(\alpha) = c_1$, $y'(\alpha) = c_2$. Choose a function g(x) s.t. $g(\alpha) = c_1$ and $g'(\alpha) = c_2$. Define

$$Y(x) = y(x) - g(x) \tag{39}$$

which satisfies $Y(\alpha) = Y'(\alpha) = 0$, and $\mathcal{L}_x Y(x) = F(x)$, where

$$F(x) = f(x) - \mathcal{L}_x g(x) = f(x) - g''(x) - p(x)g'(x) - q(x)g(x)$$
(40)

Then we can solve for Y as before and that will give us y(x) = Y(x) + g(x).

2.2.3 Homogeneous Two-Point Boundary Conditions

Consider homogeneous two-point boundary conditions $y(\alpha) = y(\beta) = 0$. A solution to eqn.(21) satisfies $y(\alpha) = 0$ is

$$y(x) = \int_{\alpha}^{x} d\tilde{x} \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) + ay_1(x) + by_2(x)$$
(41)

We choose $y_1(\alpha) = y_2(\beta) = 0$. Setting $y(\alpha) = 0$ gives

$$y(\alpha) = y_0(\alpha) + ay_1(\alpha) + by_2(\alpha) = by_2(\alpha) = 0 \quad \Rightarrow \quad b = 0$$
 (42)

Similarly, setting $y(\beta) = 0$ gives

$$y(\beta) = y_0(\beta) + ay_1(\beta) + by_2(\beta)$$

$$= -\int_{\alpha}^{\beta} d\tilde{x} \frac{y_1(\beta)y_2(\tilde{x})}{W(\tilde{x})} f(\tilde{x}) + ay_1(\beta) = 0 \quad \Rightarrow \quad a = \int_{\alpha}^{\beta} d\tilde{x} \frac{y_2(\tilde{x})}{W(\tilde{x})} f(\tilde{x})$$
(43)

which may be substituted in to the solution to give

$$y(x) = \int_{\alpha}^{x} d\tilde{x} \frac{y_{1}(\tilde{x})y_{2}(x) - y_{2}(\tilde{x})y_{1}(x)}{W(\tilde{x})} f(\tilde{x}) + ay_{1}(x)$$

$$= \int_{\alpha}^{x} d\tilde{x} \frac{y_{1}(\tilde{x})y_{2}(x) - y_{2}(\tilde{x})y_{1}(x)}{W(\tilde{x})} f(\tilde{x}) + \int_{\alpha}^{\beta} d\tilde{x} \frac{y_{2}(\tilde{x})y_{1}(x)}{W(\tilde{x})} f(\tilde{x})$$

$$= \int_{\alpha}^{x} dx \frac{y_{1}(\tilde{x})y_{2}(x)}{W(\tilde{x})} f(\tilde{x}) + \int_{x}^{\beta} dx \frac{y_{2}(\tilde{x})y_{1}(x)}{W(\tilde{x})} f(\tilde{x})$$

$$= \int_{\alpha}^{\beta} d\tilde{x} G(x, \tilde{x}) f(\tilde{x})$$

$$(44)$$

where we have defined the Green Function

$$G(x,\tilde{x}) = \begin{cases} \frac{y_1(\tilde{x})y_2(x)}{W(\tilde{x})}, & \alpha \le \tilde{x} < x\\ \frac{y_2(\tilde{x})y_1(x)}{W(\tilde{x})}, & x < \tilde{x} \le \beta \end{cases}$$

$$\tag{45}$$

Consider $G(x, \tilde{x})$ as a function of x at a fixed value of $\tilde{x} \in [\alpha, \beta]$, which has several properties

1. When $x \neq \tilde{x}$

$$\mathcal{L}_x[G(x,\tilde{x})] = 0 \tag{46}$$

2. $G(x, \tilde{x})$ is continuous at $x = \tilde{x}$

$$\lim_{\varepsilon \to 0} \left[G(x, \tilde{x}) \right]_{x = \tilde{x} - \varepsilon}^{x = \tilde{x} + \varepsilon} = \lim_{\varepsilon \to 0} \left[\frac{y_1(\tilde{x})y_2(\tilde{x} + \varepsilon)}{W(\tilde{x})} - \frac{y_2(\tilde{x})y_1(\tilde{x} - \varepsilon)}{W(\tilde{x})} \right] = 0 \tag{47}$$

3. $\frac{\partial}{\partial x}G(x,\tilde{x})$ has a unit discontinuity at $x=\tilde{x}$

$$\lim_{\varepsilon \to 0} \left[\frac{\partial G(x, \tilde{x})}{\partial x} \right]_{x = \tilde{x} - \varepsilon}^{x = \tilde{x} + \varepsilon} = \lim_{\varepsilon \to 0} \left[\frac{y_1(\tilde{x})y_2'(\tilde{x} + \varepsilon)}{W(\tilde{x})} - \frac{y_2(\tilde{x})y_1'(\tilde{x} - \varepsilon)}{W(\tilde{x})} \right]$$

$$= \frac{W(\tilde{x})}{W(\tilde{x})} = 1$$
(48)

2.3 Green Function More Generally

Let $G(x, \tilde{x})$ be a function that satisfies

$$\mathcal{L}_x[G(x,\tilde{x})] = \delta(x - \tilde{x})$$
(49)

 $\delta(x)$ is the Dirac delta-function which satisfies

- 1. $\delta(x) = 0$ when $x \neq 0$
- 2. $\delta(x) = \delta(-x)$

3.
$$\int_a^b \delta(x - x_0) f(x) dx = \begin{cases} 0, & x_0 \notin [a, b] \\ f(x_0), & x_0 \in [a, b] \end{cases}$$

 $G(x, \tilde{x})$ is called a *Green function* for the differential operator \mathcal{L}_x . If $G(x, \tilde{x})$ satisfies eqn.(49), then so does $G(x, \tilde{x}) + Y(x)$, where $\mathcal{L}_x[Y(x)] = 0$.

Now define

$$y_0(x) = \int_{\alpha}^{\beta} d\tilde{x} G(x, \tilde{x}) f(\tilde{x})$$
(50)

is a solution of $\mathcal{L}_x[y(x)] = f(x)$. Which can be verified by operating on both sides with \mathcal{L}_x , i.e.

$$\mathcal{L}_x[y_0] = \int_{\alpha}^{\beta} d\tilde{x} \mathcal{L}_x[G(x,\tilde{x})]f(\tilde{x}) = \int_{\alpha}^{\beta} d\tilde{x} \delta(x-\tilde{x})f(\tilde{x}) = f(x)$$
 (51)

f(x) is a "linear combination" of delta-function spikes at each $x = \tilde{x}$ with coefficient $f(\tilde{x})$. So y is a continuous linear combination of $G(x, \tilde{x})$ responses

$$y_0(x) = \int_{\alpha}^{\beta} d\tilde{x} G(x, \tilde{x}) f(\tilde{x})$$
 (52)

This is called *linear response*.

We can now solve for a and b using the boundary conditions that y satisfies.

2.3.1 Homogeneous Initial Conditions

The boundary conditions are $y(\alpha) = y'(\alpha) = 0$. If $G(\alpha, \tilde{x}) = G'(\alpha, \tilde{x}) = 0$, then

$$y(x) = \int_{\alpha}^{\beta} d\tilde{x} G(x, \tilde{x}) f(\tilde{x})$$
 (53)

is the solution of the ode and satisfies the boundary conditions. Now, let's look for the Green function with the right boundary conditions.

1. For $x < \tilde{x}$, $\mathcal{L}_x[G(x,\tilde{x})] = 0$. $G(x,\tilde{x}) = 0$ is a solution of the homogeneous equation that satisfies the boundary conditions that $G(\alpha,\tilde{x}) = G'(\alpha,\tilde{x}) = 0$. So for $x < \tilde{x}$

$$G(x, \tilde{x}) = 0 \tag{54}$$

2. For $x \geq \tilde{x}$, $\mathcal{L}_x[G(x,\tilde{x})] = 0$. $G(x,\tilde{x})$ equals some linear combination of $y_1(x)$ and $y_2(x)$

$$G(x,\tilde{x}) = A(\tilde{x})y_1(x) + B(\tilde{x})y_2(x)$$
(55)

We can find A and B by using the properties of G:

(i) G is continuous at $x = \tilde{x}$

$$A(\tilde{x})y_1(\tilde{x}) + B(\tilde{x})y_2(\tilde{x}) = 0$$
 (56)

(ii) G' has a unit discontinuity at $x = \tilde{x}$

$$A(\tilde{x})y_1'(\tilde{x}) + B(\tilde{x})y_2'(\tilde{x}) = 0$$
(57)

The solution is

$$A(\tilde{x}) = -\frac{y_x(\tilde{x})}{W(\tilde{x})}, \qquad B(\tilde{x}) = \frac{y_1(\tilde{x})}{W(\tilde{x})}$$
(58)

where W is the Wronskian of y_1 and y_2 .

So we have

$$G(x, \tilde{x}) = \begin{cases} 0, & x < \tilde{x} \\ \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})}, & x > \tilde{x} \end{cases}$$
 (59)

which agrees with that calculated before.

2.3.2 Homogeneous Two-Point Boundary Conditions

The boundary conditions are $y(\alpha) = y(\beta) = 0$. The Green Function should satisfies

$$G(\alpha, \tilde{x}) = G(\beta, \tilde{x}) = 0 \tag{60}$$

We assume y_1 and y_2 are linear independent solutions of homogeneous equation, and we choose $y_1(\alpha) = y_2(\beta) = 0$.

$$G(x, \tilde{x}) = \begin{cases} A(\tilde{x})y_1(x) + B(\tilde{x})y_2(x), & \alpha < x < \tilde{x} \\ C(\tilde{x})y_1(x) + D(\tilde{x})y_2(x), & \tilde{x} < x < \beta \end{cases}$$
(61)

1. Boundary conditions: $G(\alpha, \tilde{x}) = G(\beta, \tilde{x}) = 0$

$$A(\tilde{x})y_1(\alpha) + B(\tilde{x})y_2(\alpha) = B(\tilde{x})y_2(\alpha) = 0 \quad \Rightarrow \quad B(\tilde{x}) = 0$$
 (62)

$$C(\tilde{x})y_1(\beta) + D(\tilde{x})y_2(\beta) = C(\tilde{x})y_1(\beta) = 0 \quad \Rightarrow \quad C(\tilde{x}) = 0$$
 (63)

so we have

$$G(x, \tilde{x}) = \begin{cases} A(\tilde{x})y_1(x), & \alpha < x < \tilde{x} \\ D(\tilde{x})y_2(x), & \tilde{x} < x < \beta \end{cases}$$
 (64)

2. Continuity of G and unit discontinuity of G' at $x = \tilde{x}$

$$A(\tilde{x})y_1(\tilde{x}) - D(\tilde{x})y_2(\tilde{x}) = 0$$
(65)

$$A(\tilde{x})y_1'(\tilde{x}) - D(\tilde{x})y_2'(\tilde{x}) = 0$$
(66)

so we have

$$A(\tilde{x}) = \frac{y_2(\tilde{x})}{W(\tilde{x})}, \qquad D(\tilde{x}) = \frac{y_1(\tilde{x})}{W(\tilde{x})}$$
(67)

The final result

$$G(x, \tilde{x}) = \begin{cases} \frac{y_2(\tilde{x})y_1(x)}{W(\tilde{x})}, & \alpha < x < \tilde{x} \\ \frac{y_1(\tilde{x})y_2(x)}{W(\tilde{x})}, & \tilde{x} < x < \beta \end{cases}$$

$$(68)$$

which agrees with that calculated before.

2.3.3 Higher Dimensions, More Variables

Consider a second order linear differential operator \mathcal{L} on function $y(x_1, x_2, x_3)$, then

$$\mathcal{L}y = f(x_1, x_2, x_3) \tag{69}$$

and

$$\mathcal{L}G(\underline{x},\underline{\tilde{x}}) = \delta^{(3)}(\underline{x} - \underline{\tilde{x}}) = \delta(x_1 - \tilde{x}_1)\delta(x_2 - \tilde{x}_2)\delta(x_3 - \tilde{x}_3)$$
(70)

Let *R* be a 3-d region in 3-d Euclidean space

$$\int_{R} d\tilde{x}_{1} d\tilde{x}_{2} \delta^{(2)}(\underline{x} - \underline{\tilde{x}}) f(\underline{\tilde{x}}) = \begin{cases} f(\underline{x}), & \underline{x} \in R \\ 0 & \underline{x} \notin R \end{cases}$$
(71)

Example. The most famous example is

$$\mathcal{L} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \nabla^2$$
 (72)

and the Green function satisfies

$$\nabla^2 G(\underline{x}, \underline{\tilde{x}}) = \delta(\underline{x} - \underline{\tilde{x}}) \tag{73}$$

Consider the Poisson equation for the scalar electric potential $\phi(\underline{x})$ in terms of the scalar charge density $\rho(\underline{x})$:

$$\nabla^2 \phi(\underline{x}) = -\frac{\rho(\underline{x})}{\varepsilon} \tag{74}$$

and

$$\phi(x) = \int d\underline{\tilde{x}} G(\underline{x}, \underline{\tilde{x}}) \left[-\frac{\rho(\underline{\tilde{x}})}{\varepsilon} \right]$$
 (75)

is a solution of Poisson's equation. The Green function for the Poisson equation that satisfying the boundary condition $G(\underline{x}, \underline{\tilde{x}}) \to 0$ as $|\underline{x}| \to \infty$ is

$$G(\underline{x}, \underline{\tilde{x}}) = \frac{1}{4\pi |x - \tilde{x}|} \tag{76}$$

where $|\underline{x} - \underline{\tilde{x}}| = \sqrt{(x_1 - \tilde{x}_1)^2 + (x_2 - \tilde{x}_2)^2 + (x_3 - \tilde{x}_3)^2}$.

3 Hilbert Spaces

Definition. A Hilbert space is an infinite dimensional complex vector space with inner product $\langle \cdot, \cdot \rangle$ and a infinite countable orthonormal basis $\{u_1, u_2, u_3, \cdots\}$. The Hilbert space we will look at in this chapter will be a vector space of complex function of a real variable $x \in [a, b]$ with

1. an inner product

$$\langle f, g \rangle = \int_{a}^{b} f^{*}(x)g(x)\mathrm{d}x$$
 (77)

Functions f(x) and g(x) are orthogonal if $\langle f, g \rangle = 0$. The *norm* of f is given by $||f|| = \sqrt{\langle f, f \rangle}$, and f(x) may be normalised in $\hat{f} = f/||f||$. If $\langle y_i, y_j \rangle = \delta_{ij}$, then the set of $\{y_1, y_2, y_3, \dots\}$ is orthogonal.

2. Let $\{y_1, y_2, y_3, \dots\}$ be an orthogonal basis, then any function $f(x) \in \mathcal{H}$ can be expanded

$$f(x) = \sum_{i=1}^{\infty} f_i y_i(x), \quad f_i \in \mathbb{C}$$
 (78)

Then we have

$$\langle y_k, f \rangle = \langle y_k, \sum_{i=1}^{\infty} f_i y_i \rangle = \sum_{i=1}^{\infty} f_i \langle y_k, y_i \rangle = \sum_{i=1}^{\infty} f_i \delta_{ik} = f_k$$
 (79)

3.1 Sturm-Liouville Theory

The theory of inhomogeneous differential equations of form $\mathcal{L}y(x) = f(x)$ on $x \in [a, b]$ where \mathcal{L} is second order, linear and **self-adjoint**.

3.1.1 Self-Adjoint Differential Operators

Consider

$$\mathcal{L} = -\frac{\mathrm{d}}{\mathrm{d}x} \left[\rho(x) \frac{\mathrm{d}}{\mathrm{d}x} \right] + \sigma(x)$$
 (80)

and

$$\mathcal{L}y = -\frac{\mathrm{d}}{\mathrm{d}x} \left(\rho \frac{\mathrm{d}y}{\mathrm{d}x} \right) + \sigma y = -(\rho y')' + \sigma y \tag{81}$$

where $\rho(x)$ and $\sigma(x)$ are real valued and defined on $x \in [a,b]$ and $\rho(x) > 0$ on $x \in (a,b)$. Such an operator is said to be in *self-adjoint form*¹.

Definition. A second order linear differential operator \mathcal{D} is self-adjoint on Hilbert space \mathcal{H} if

¹being in self-adjoint form does not mean that a differential operator is self-adjoint, that depend on the operator and the specific Hilbert space.

c.f. the definition of a Hermitian matrix $M: M_{ij} = M_{ii}^*$.

Consider \mathcal{L} as in eqn.(80),

$$\langle u, \mathcal{L}v \rangle = \int_{a}^{b} u^{*} \left[-(\rho v')' + \sigma v \right] dx$$

$$= -u^{*} \rho v' \Big|_{a}^{b} + \int_{a}^{b} \left(u^{*'} \rho v' + u^{*} \sigma v \right) dx$$

$$= -u^{*} \rho v' \Big|_{a}^{b} + u^{*'} \rho v \Big|_{a}^{b} + \int_{a}^{b} \left(-(u^{*'} \rho)' v + u^{*} \sigma v \right) dx$$

$$= \left(-u^{*} \rho v' + u^{*'} \rho v \right) \Big|_{a}^{b} + \int_{a}^{b} \left(-(u^{*'} \rho)' + u^{*} \sigma \right) v dx$$

$$= \left(-u^{*} \rho v' + u^{*'} \rho v \right) \Big|_{a}^{b} + \left[\int_{a}^{b} \left(-(u' \rho)' + u \sigma \right) v^{*} dx \right]^{*}$$

$$= \left(-u^{*} \rho v' + u^{*'} \rho v \right) \Big|_{a}^{b} + \left\langle v, \mathcal{L}u \right\rangle^{*}$$
(83)

So \mathcal{L} is self-adjoint on \mathcal{H} if

$$\rho(u^{*'}v - u^{*}v')\Big|_{a}^{b} = 0 \tag{84}$$

3.1.2 Boundary Conditions

- 1. if $\rho(a) = \rho(b) = 0$ and u(a)u(b) is finite for all $u \in \mathcal{H}$, then \mathcal{L} is self-adjoint.
- 2. if u(a) = u(b) and u'(a) = u'(b) for all $u \in \mathcal{H}$, and $\rho(a) = \rho(b)$, then \mathcal{L} is self-adjoint. \mathcal{H} is set of functions of periodic boundary conditions.
- 3. If u(a) = u(b) = 0 for all $u \in \mathcal{H}$, then \mathcal{L} is self-adjoint. This is a special case of

$$\begin{cases}
C_1 u(a) + C_2 u'(a) = 0 \\
D_1 u(b) + D_2 u'(b) = 0
\end{cases}$$
(85)

Note that these examples of boundary conditions that work are preserved under taking linear combinations

3.1.3 Weight Functions

Any second order linear differential operator can be put into self-adjoint form. Consider the most general operator

$$\tilde{\mathcal{L}} = -\frac{\mathrm{d}}{\mathrm{d}x} \left(A(x) \frac{\mathrm{d}}{\mathrm{d}x} \right) - B(x) \frac{\mathrm{d}}{\mathrm{d}x} + C(x)$$
(86)

where A, B, C are real and A(x) > 0 for $x \in [a, b]$.

Claim that there exists a function w(x) > 0 such that $w\tilde{\mathcal{L}}$ can be written in self-adjoint form i.e.

$$w(x) [-(Ay')' - By' + Cy] = -(\rho y')' + \sigma y$$
(87)

rearranging this

$$-w(Ay')' - Bwy' + Cwy = -(\rho y')' + \sigma y \tag{88}$$

so we have

$$\begin{cases}
-(Awy')' + w'Ay' - Bwy' = -(\rho y')' \\
Cwy = \sigma y
\end{cases}$$
(89)

then

$$\frac{w'}{w} = \frac{B}{A}, \qquad Aw = \rho, \qquad Cw = \sigma \tag{90}$$

We choose w(x) such that

$$w(x) = \exp\left[\int_{a}^{x} \frac{B(\tilde{x})}{A(\tilde{x})} d\tilde{x}\right]$$
 (91)

where w(a) = 1.

Definition. The inner product with weight w

$$\langle f, g \rangle_w = \langle f, wg \rangle = \int_a^b f^*(x) w(x) g(x) dx = \langle wf, g \rangle$$
 (92)

w is real.

3.1.4 Eigenfunctions and Eigenvalues

Consider the inhomogeneous eigenfunction equation

$$\tilde{\mathcal{L}}y = \lambda y \tag{93}$$

we may define an operator in self-adjoint form $\mathcal{L}=w\tilde{\mathcal{L}}$ and eigenfunction equation becomes

$$\boxed{\mathcal{L}y = \lambda wy} \tag{94}$$

A solution is called an eigenfunction of \mathcal{L} with eigenvalue λ and weight w(x). We claim that

- 1. The eigenvalues of eqn.(94) are real.
- 2. The eigenfunctions of eqn. (94) with distinct eigenvalues are orthogonal.

Consider two eigenfunctions, y_i and y_j of $\tilde{\mathcal{L}}$ with eigenvalues λ_i and λ_j respectively. They are also eigenfunctions of \mathcal{L} with eigenvalues λ_i and λ_j and weight w. Then we have

$$\mathcal{L}y_i = \lambda_i w y_i \tag{95}$$

$$\langle y_j, \mathcal{L}y_i \rangle = \lambda_i \langle y_j, wy_i \rangle \tag{96}$$

$$\langle y_j, \mathcal{L}y_i \rangle^* = \lambda_i^* \langle y_j, wy_i \rangle^*$$
 (take complex conjugate) (97)

$$\langle y_i, \mathcal{L}y_j \rangle = \lambda_i^* \langle y_i, wy_j \rangle = \lambda_i^* \langle y_i, y_j \rangle_w$$
 (use self-adjointness) (98)

$$\mathcal{L}y_j = \lambda_j w y_j \tag{99}$$

$$\langle y_i, \mathcal{L}y_j \rangle = \lambda_j \langle y_i, wy_j \rangle = \lambda_j \langle y_i, y_j \rangle_w \tag{100}$$

Compare eqn. (98) and eqn. (100), we find

$$(\lambda_i^* - \lambda_i)\langle y_i, y_i \rangle_w = 0 \tag{101}$$

• For i = j we have

$$(\lambda_i^* - \lambda_i) \|y_i\|_w^2 = 0 \tag{102}$$

so, if we have non-zero eigenfunctions, then $\lambda_i^* = \lambda_i$, *i.e.*, the eigenvalues are real.

• For $i \neq j$ we have

$$(\lambda_i - \lambda_j) \langle y_i, y_j \rangle_w = 0 \tag{103}$$

so, if we are considering distinct eigenvalues, then $\langle y_i, y_j \rangle_w = 0$, i.e., the eigenfunctions are orthogonal with weight w(x).

3.1.5 Eigenfunction Expansions

Theorem. The eigenvalues of a self-adjoint operator with w form a discrete, infinite sequence $\lambda_1, \lambda_2, \lambda_3, \cdots$ such that $|\lambda_n| \to \infty$ as $n \to \infty$, and that the corresponding eigenfunctions with weight w, $f_1, f_2, f_3 \cdots$ form a *complete orthonormal basis* for functions on [a, b] in the Hilbert space. So any function $g \in \mathcal{H}$ can be expanded as

$$g(x) = \sum_{n} g_n f_n(x), \quad g_n \in \mathbb{C}$$
 (104)

where

$$g_n = \langle f_n, g \rangle_{\omega} = \int_a^b f_n^*(x) w(x) g(x) dx$$
 (105)

Substituting into the expansion we find

$$g(x) = \sum_{n} \int_{a}^{b} d\tilde{x} \left[f_{n}^{*}(\tilde{x}) w(\tilde{x}) g(\tilde{x}) \right] f_{n}(x)$$

$$= \int_{a}^{b} d\tilde{x} g(\tilde{x}) \left[w(\tilde{x}) \sum_{n} f_{n}(x) f_{n}^{*}(\tilde{x}) \right]$$

$$= \int_{a}^{b} d\tilde{x} \delta(x - \tilde{x}) g(\tilde{x})$$
(106)

where

$$\delta(x - \tilde{x}) = w(\tilde{x}) \sum_{n} f_n(\tilde{x}) f_n^*(\tilde{x})$$
(107)

Let $u \in \mathcal{H}$, consider the expression

$$\int_{a}^{b} |u|^{2} \omega dx = \langle u, u \rangle_{w} = \langle \sum_{n} u_{n} f_{n}(x), \sum_{m} u_{m} f_{m}(x) \rangle_{w}$$

$$= \sum_{n,m} u_{n}^{*} u_{m} \langle f_{n}, f_{m} \rangle_{w} = \sum_{n,m} u_{n}^{*} u_{m} \delta_{nm} = \sum_{n} |u_{n}|^{2}$$

$$(108)$$

which is *Parseval's identity* in the case with a weight function w(x)

$$\langle u, u \rangle_w = \sum_n |u_n|^2 \tag{109}$$

3.1.6 Green Functions Revisited

If $\{y_n\}$ are a set of orthonormal eigenfunctions of self-adjoint operator \mathcal{L} with weight w with corresponding eigenvalues $\{\lambda_n\}$, then the Green function for \mathcal{L} is given by

$$G(x,\tilde{x}) = \sum_{n} \frac{y_n(x)y_n^*(\tilde{x})}{\lambda_n}$$
(110)

To prove this, we apply \mathcal{L} to $G(x, \tilde{x})$

$$\mathcal{L}_{x}[G(x,\tilde{x})] = \sum_{n} \frac{\mathcal{L}_{x}[y_{n}(x)]y_{n}^{*}(\tilde{x})}{\lambda_{n}}$$

$$= \sum_{n} w(x)y_{n}(x)y_{n}^{*}(\tilde{x})$$

$$= \frac{\omega(x)}{\omega(\tilde{x})} \left[\omega(\tilde{x}) \sum_{n} y_{n}(x)y_{n}^{*}(\tilde{x}) \right]$$

$$= \delta(x - \tilde{x}) \quad \Box$$
(111)

3.1.7 Eigenfunction Expansions for Solving ODEs

As an example, consider the differential equation

$$\mathcal{L}y - \nu y = f \tag{112}$$

with some boundary conditions. \mathcal{L} is a self-adjoint operator with weight function w=1 and $\{y_n\}$ are eigenfunctions. Suppose \mathcal{L} has eigenvalues λ_n , and corresponding eigenfunctions $\{y_n\}$, satisfying the same boundary conditions. Let

$$y(x) = \sum_{n} a_n y_n(x), \qquad f(x) = \sum_{n} f_n y_n(x)$$
 (113)

Substituting into the original equation, we find

$$\mathcal{L}\sum_{n} a_{n}y_{n} - \nu \sum_{n} a_{n}y_{n} = \sum_{n} f_{n}y_{n}$$

$$\Rightarrow \sum_{n} (a_{n}\lambda_{n} - \nu a_{n})y_{n} = \sum_{n} f_{n}y_{n}$$

$$\Rightarrow (a_{n}\lambda_{n} - \nu a_{n}) = f_{n}$$
(114)

So that

$$a_n = \frac{f_n}{\lambda_n - \nu}, \qquad (\lambda_n \neq \nu)$$
 (115)

so that the solution is given by

$$y(x) = \sum_{n} \frac{f_n}{\lambda_n - \nu} y_n(x) \tag{116}$$

3.2 Legendre Polynomials

3.2.1 Two Examples

Example. Let

$$\mathcal{L} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \qquad x \in [0, 2\pi R] \tag{117}$$

with boundary conditions $y(0)=y(2\pi R)=0$. Then the eigenfunction equation becomes

$$-y_n'' = \lambda_n y_n \tag{118}$$

and the eigenfunctions and the corresponding eigenvalues are

$$y_n = \sin\left(\frac{n}{2R}x\right), \qquad \lambda_n = \left(\frac{n}{2R}\right)^2, \qquad n = 1, 2, 3, \dots$$
 (119)

Example. Let

$$\mathcal{L} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \qquad x \in [0, 2\pi R]$$
 (120)

with boundary conditions $y(0) = y(2\pi R)$ and $y'(0) = y'(2\pi R)$.

$$-y_m'' = \lambda_m y_m \tag{121}$$

and the eigenfunctions and the corresponding eigenvalues are

$$y_m = \exp\left(i\frac{m}{R}x\right), \qquad \lambda_m = \left(\frac{m}{2R}\right)^2, \qquad m \in \mathbb{Z}$$
 (122)

When m=0, there's the extra 'zero mode' of y_0 is a constant with eigenvalue 0.

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left[(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}y\right] = \lambda y \tag{123}$$

Assume that eigenfunctions of eqn.(123) are polynomials

$$y_n(x) = x^{m_n} + a_{m-1}x^{m_n-1} + \dots + a_1x + a_0$$
(124)

substituting this to the eigenfunction equation, we have

$$m_n(m_n+1) = \lambda \tag{125}$$

So eigenvalues take form

$$\lambda = l(l+1), \qquad l \in \mathbb{N} \tag{126}$$

We can label the eigenfunctions by l

- $l = 0, y_0(x) = 1$
- $l = 1, y_1(x) = x + a_0$
- $l=2, y_2(x)=x^2+a_1x+a_0$

$$\int_{-1}^{1} y_{l}^{*}(x) y_{l'}(x) \mathrm{d}x = \delta_{ll'}$$
 (127)

3.2.2 Legendre's Equation

Legendre's equation

$$(1-x^2)y'' - 2xy' + l(l+1)y = 0$$
 with $x \in [-1, 1]$ (128)

arises is a number of contexts in science, for example in the solution of Laplace's equation in spherical coordinates. This equation can be put into the form of a self-adjoint eigenvalue problem with $\rho=1-x^2$, $\sigma=0$, w=1 and $\lambda=l(l+1)$.

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left[(1-x^2)y'\right] = l(l+1)y \tag{129}$$

or

$$\mathcal{L}y = l(l+1)y \tag{130}$$

where

$$\mathcal{L} = -\frac{\mathrm{d}}{\mathrm{d}x} \left[(1 - x^2) \frac{\mathrm{d}}{\mathrm{d}x} \right] \tag{131}$$

is self-adjoint on a Hilbert space of functions that are finite at ± 1 . Assume that eigenfunctions of eqn.(129) are polynomials

$$y_n(x) = x^{m_n} + a_{m_n-1}x^{m_n-1} + \dots + a_1x + a_0$$
(132)

Substituting the polynomial solution y_n into eqn.(129), then thinking about equation coefficients of partial of x. The highest power m_n satisfies the relation

$$m_n(m_n+1) = \lambda \tag{133}$$

So eigenvalues take form

$$\lambda = l(l+1), \qquad l \in \mathbb{N} \tag{134}$$

and can label eigenfunctions by l

- $l = 0, y_0(x) = 1$
- $l = 1, y_1(x) = x + a_0$
- $l=2, y_2(x)=x^2+a_1x+a_0$

3.3 Spherical Harmonics

Laplace's equation in spherical coordinates is given by

$$\nabla^2 f(r,\theta,\phi) = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial^2 f}{\partial \phi^2}$$
(135)

If we take

$$f(r,\theta,\phi) = r^l e^{im\phi} \Theta(\theta)$$
 (136)

as an ansatz, where $l \in \mathbb{N}$ and $m \in \mathbb{Z}$, then Laplace's equation becomes

$$l(l+1)e^{im\phi}\Theta(\theta) + \frac{e^{im\phi}}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) - \frac{\Theta}{\sin\theta}m^2e^{im\phi} = 0$$
 (137)

Rearrange this, we have

$$\sin^2 \theta l(l+1) + \frac{\sin \theta}{\Theta} \frac{\mathrm{d}}{\mathrm{d}\theta} \left(\sin \theta \frac{\mathrm{d}\Theta}{\mathrm{d}\theta} \right) = m^2$$
 (138)

Let $u = \cos \theta$ and $\Theta(\theta) = P(u)$, where $u \in [-1, 1]$, we have

$$\frac{\mathrm{d}}{\mathrm{d}\theta} = \frac{\mathrm{d}}{\mathrm{d}u} \frac{\mathrm{d}u}{\mathrm{d}\theta} = -\sin\theta \frac{\mathrm{d}}{\mathrm{d}u} \tag{139}$$

Then the equation becomes

$$-[(1-u^2)P']' + \frac{m^2}{1-u^2}P = l(l+1)P$$
(140)

with $\rho=1-u^2$, $\sigma=\frac{m^2}{1-u^2}$, w=1 and $\lambda=l(l+1)$. Now the differential operators depend on m, and there will be a different set of indefinite solutions for each m. This can show that we get non-singular solutions if $l\in\mathbb{N}$ and $m\in[-l,l]$. The solutions are called associated Legendre polynomials $P_l^m(u)$, which is a basis set for functions of u on [-1,1].

The orthogonality

$$\int_{-1}^{1} P_{l}^{m}(u) P_{l'}^{m}(u) du = \frac{2(l+m)!}{(2l+1)(l-m)} \delta_{ll'}$$
(141)

Similarly, the equation can be expressed as

$$-[(1-u^2)P']' - l(l+1)P = -\frac{m^2}{1-u^2}P$$
 (142) self-adjoint form

with $\rho=1-u^2$, $\sigma=-l(l+1)$ and $w=\frac{1}{1-u^2}$ This show that

$$\int_{-1}^{1} \frac{P_l^m(u)P_l^{m'}(u)}{1-u^2} du = \frac{(l+m)!}{m(l-m)} \delta_{mm'}$$
(143)

Finally we get

$$Y_l^m = (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos \theta) e^{im\phi}, \quad l \in \mathbb{N}, -l \le m \le l$$
 (144)

they are solutions of $\nabla^2 Y_l^m = 0$, and form an orthogonal basis of function on \mathbf{S}^2

$$\delta_{ll'}\delta_{mm'} = \int_0^{2\pi} \int_0^{\pi} Y_l^m(\theta,\phi) Y_{l'}^{m'}(\theta,\phi) \sin\theta d\theta d\phi \tag{145}$$

So any function f can be expressed as

$$f(\theta,\phi) = \sum_{l} \sum_{m=-l}^{l} f_{lm} Y_l^m(\theta,\phi)$$
(146)

where

$$f_{lm} = \int_{\mathbf{S}^2} Y_l^{m*} f d\Omega \tag{147}$$

4 Integral Transforms

4.1 Fourier Series

Consider f(x) has a period of $2\pi R$, we can express f(x) as

$$f(x) = \sum_{n = -\infty}^{\infty} f_n y_n(x)$$
(148)

where

$$y_n(x) = \frac{1}{\sqrt{2\pi R}} e^{inx/R} \tag{149}$$

and we have

$$\langle y_n, y_m \rangle = \int_0^{2\pi R} y_n^* y_m \mathrm{d}x = \delta_{nm}$$
 (150)

We choose $x \in [-\pi R, \pi R]$, then

$$f_n = \int_{-\pi R}^{\pi R} y_n^*(x) f(x) dx$$

$$= \frac{1}{\sqrt{2\pi R}} \int_{-\pi R}^{\pi R} e^{-inx/R} f(x) dx$$

$$= \frac{1}{\sqrt{2\pi R}} \int_{-\pi R}^{\pi R} e^{-ik_n x} f(x) dx$$
(151)

where $k_n = n/R$, $x \in (-\infty, \infty)$. Let $R \to \infty$ and k_n take the real continuous values from $-\infty$ to ∞ , we define that

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} f(x) dx$$
 (152)

for f satisfying $\int_{-\infty}^{\infty} |f| \mathrm{d}x$ is finite. $\tilde{f}(k)$ is the Fourier transform of f(x).

4.2 Fourier Transforms

4.2.1 Definition and Notation

Definition. Fourier transform

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$
(153)

The inverse Fourier transform is defined as

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx} dk$$
(154)

In other words, this operation on $\tilde{f}(k)$ is the inverse Fourier transform and we can define

$$FT^{-1}[FT(f)] = f \quad \Rightarrow \quad FT^{-1}FT = 1$$
 (155)

4.2.2 Dirac Delta-Function

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx} dk$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x') e^{-ikx'} dx' \right] e^{ikx} dk$$

$$= \int_{-\infty}^{\infty} f(x') \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} dk \right] dx'$$

$$= \int_{-\infty}^{\infty} f(x') \delta(x-x') dx'$$
(156)

where we have defined the Dirac delta-function

$$\delta(x - x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x - x')} dk$$
(157)

4.2.3 Properties of the Fourier Transform

1. If f(x) is a real function $[f(x)]^* = f(x)$

$$\tilde{f}^*(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i(-k)x} f^*(x) dx = \tilde{f}(-k)$$
 (158)

• If f(x) is an even function f(-x) = f(x), then $\tilde{f}(x)$ is a pure real function. **Proof.** Define y = -x, then

$$\tilde{f}^*(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-iky} f(-y) d(-y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-iky} f(y) dy = \tilde{f}(k)$$
 (159)

• If f(x) is an off function f(-x) = -f(x), then $\tilde{f}(x)$ is a pure imaging function.

Proof. Define y = -x, then

$$\tilde{f}^*(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-iky} f(-y) d(-y) = -\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-iky} f(y) dy = -\tilde{f}(k)$$
(160)

2. Differentiation

$$TF[f^{(n)}(x)] = (ik)^n \tilde{f}(k)$$
(161)

Proof. Consider the first order derivative

$$TF[f'(x)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-ikx} f'(x)$$

$$= \frac{1}{\sqrt{2\pi}} \left[f(x) e^{-ikx} \right]_{-\infty}^{\infty} - \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx f(x) (-ik) e^{-ikx}$$

$$= ik \tilde{f}(k)$$
(162)

3. Multiplication by x

$$FT[xf(x)] = i\frac{\mathrm{d}}{\mathrm{d}x}\tilde{f}(k) \tag{163}$$

4. Rigid shift of coordinate

$$FT[f(x-a)] = e^{-ika}\tilde{f}(k)$$
(164)

Proof. Define y = x - a, then

$$\operatorname{FT}[f(x-a)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} f(x-a) dx$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ika} e^{-ik(x-a)} f(x-a) d(x-a)$$

$$= \frac{1}{\sqrt{2\pi}} e^{-ika} \int_{-\infty}^{\infty} e^{-iky} f(y) dy = e^{-ika} \tilde{f}(k)$$
(165)

4.2.4 Parseval's Theorem

Parseval's theorem for Fourier transforms states that

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = \int_{-\infty}^{\infty} |\tilde{f}(k)|^2 dk$$
(166)

Proof.

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = \int_{-\infty}^{\infty} f(x) f^*(x) dx$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \tilde{f}(k) \tilde{f}^*(k') e^{i(k-k')x} \right] dx$$

$$= \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \tilde{f}(k) \tilde{f}^*(k') \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k-k')x} dx \right]$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{f}(k) \tilde{f}^*(k') \delta(k-k') dk dk'$$

$$= \int_{-\infty}^{\infty} \tilde{f}(k) \tilde{f}^*(k) dk = \int_{-\infty}^{\infty} |\tilde{f}(k)|^2 dk$$
(167)

4.2.5 Convolution Theorem

The convolution of f and g is defined as

$$f * g = \int_{-\infty}^{\infty} f(y)g(x - y)dy$$
(168)

with claims

1.
$$f * g = g * f$$

2. $f * \delta = f$

The convolution theorem can be stated in two, equivalent forms.

1.

$$FT(f * g) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-ikx} \int_{-\infty}^{\infty} dy f(y) g(x - y)$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dy e^{-iky} f(y) \int_{-\infty}^{\infty} dx e^{-ik(x-y)} g(x - y)$$

$$= \sqrt{2\pi} \tilde{f}(k) \tilde{g}(k) = \sqrt{2\pi} FT[f] FT[g]$$
(169)

2.

$$FT[f(x)g(x)] = \frac{1}{\sqrt{2\pi}}\tilde{f}(k) * \tilde{g}(k)$$
(170)

4.2.6 Examples of Fourier Transform

1. Constant function f(x) = 1

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} dx = \sqrt{2\pi} \delta(k)$$
(171)

2. Single frequency/wavenumber mode $f(x) = e^{ik_0x}$

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ik_0 x} e^{-ikx} dx = \sqrt{2\pi} \delta(k - k_0)$$
(172)

3. Dirac delta-function $f(x) = \delta(x - x_0)$

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(x - x_0) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} e^{-ikx_0}$$
 (173)

4. Gaussian function $f(x) = \frac{1}{\sigma(2\pi)^{1/4}} e^{-x^2/4\sigma^2}$

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma(2\pi)^{1/4}} \int_{-\infty}^{\infty} e^{-x^2/4\sigma^2} e^{-ikx} dx
= \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma(2\pi)^{1/4}} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{4\sigma^2} - ikx\right) dx
= \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma(2\pi)^{1/4}} \int_{-\infty}^{\infty} \exp\left[-\frac{1}{4\sigma^2} (x + ik2\sigma)^2 - k^2\sigma^2\right] dx
= \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma(2\pi)^{1/4}} e^{-k^2\sigma^2} \int_{-\infty}^{\infty} \exp\left[-\frac{1}{4\sigma^2} (x + ik2\sigma)^2\right] dx
= \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma(2\pi)^{1/4}} e^{-k^2\sigma^2} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{4\sigma^2} x'^2\right) dx'
= \frac{\sqrt{2\sigma}}{(2\pi)^{\frac{1}{4}}} e^{-k^2\sigma^2}$$
(174)

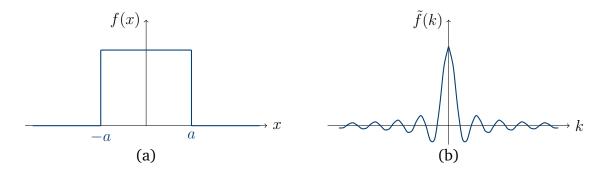


Figure 2: Top-hat function.

5. Top-hat function
$$f(x) = \begin{cases} 1 & |x| < a \\ 0 & |x| \ge a \end{cases}$$

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-a}^{a} e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \left[-\frac{1}{ik} e^{-ikx} \right]_{-a}^{a}$$

$$= \sqrt{\frac{2}{\pi}} \frac{\sin(ka)}{k} = a\sqrt{\frac{2}{\pi}} \operatorname{sinc}(ak)$$

$$(175)$$

4.3 The Applications of Fourier Transforms in Physics

4.3.1 Diffraction Through an Aperture

The geometry for Fraunhofer diffraction see Fig.3(a). For small values of θ we have $\theta \approx \sin \theta \approx \tan \theta = \frac{X}{D}$. The aperture function is given by a top-hat

$$h(x) = \begin{cases} 1 & |x| < \frac{a}{2} \\ 0 & |x| \ge \frac{a}{2} \end{cases}$$
 (176)

so we have

$$\tilde{h}(k) = \frac{a}{\sqrt{2\pi}} \operatorname{sinc}\left(\frac{ak}{2}\right) \tag{177}$$

The intensity I(k) of light observed in the diffraction pattern is the square of the Fourier transform of the aperture function f(x)

$$I(x = X) = I\left(k_x = \frac{2\pi X}{\lambda D}\right) = |\tilde{h}(k_x)|^2 = \frac{a^2}{2\pi} \operatorname{sinc}^2\left(\frac{a\pi X}{2\lambda D}\right)$$
(178)

4.3.2 Double Slit Diffraction

The aperture function is given by

$$h(x) = f(x)g(x) \tag{179}$$

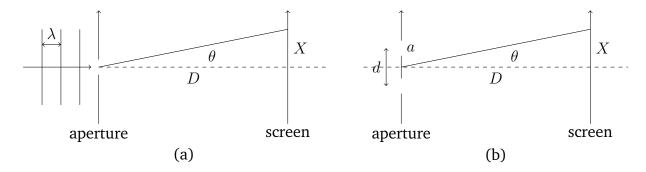


Figure 3: Geometry for Fraunhofer diffraction. (a) Diffraction through an aperture. (b) Double slit diffraction.

where

$$f(x) = \delta\left(x - \frac{d}{2}\right) + \delta\left(x + \frac{d}{2}\right) \tag{180}$$

and g(x) is single aperture function. And

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-ikx} \left[\delta \left(x - \frac{d}{2} \right) + \delta \left(x + \frac{d}{2} \right) \right]$$

$$= \frac{1}{\sqrt{2\pi}} \left(e^{-ikd/2} + e^{ikd/2} \right) = \sqrt{\frac{2}{\pi}} \cos \left(\frac{kd}{2} \right)$$
(181)

so we have

$$\begin{aligned} \text{TF}(f*g) &= \sqrt{2\pi} \tilde{f}(k) \tilde{g}(k) \\ &= \sqrt{2\pi} \sqrt{\frac{2}{\pi}} \cos\left(\frac{kd}{2}\right) \frac{a}{\sqrt{2\pi}} \text{sinc}\left(\frac{ak}{2}\right) \\ &= \sqrt{\frac{2}{\pi}} a \text{sinc}\left(\frac{ak}{2}\right) \cos\left(\frac{kd}{2}\right) \end{aligned} \tag{182}$$

and the intensity on the screen is given by

$$I(k) = \frac{2a^2}{\pi} \operatorname{sinc}^2\left(\frac{ak}{2}\right) \cos^2\left(\frac{kd}{2}\right) \tag{183}$$

4.3.3 Diffusion Equation

Consider an infinite, one-dimensional conducting bar. The flow of heat is determined by the diffusion equation

$$\frac{\partial \theta}{\partial t} = D \frac{\partial^2 \theta}{\partial x^2} \tag{184}$$

where θ is the heat distribution. The boundary conditions on this problem is $\theta(\pm \infty, t = 0)$ and $\theta(x, t = 0) = \delta(x)$.

$$\frac{\partial}{\partial t}\tilde{\theta}(k,t) = D(ik)^2\tilde{\theta}(k,t) = -Dk^2\tilde{\theta}(k,t) \tag{185}$$

the solution is

$$\tilde{\theta}(k,t) = \tilde{\theta}(k,0)e^{-Dk^2t} = \text{FT}[\delta(x)]e^{-Dk^2t} = \frac{1}{\sqrt{2\pi}}e^{-Dk^2t}$$
 (186)

So we have

$$\theta(x,t) = \operatorname{FT}^{-1}[\tilde{\theta}(k,t)]$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ikx} e^{-Dk^2t}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \exp\left[-Dt \left(k - \frac{ix}{2Dt}\right)^2 - \frac{x^2}{4Dt}\right] dk$$

$$= \frac{1}{2\pi} e^{-x^2/4Dt} \int_{-\infty}^{\infty} e^{-Dtq^2} dq$$

$$= \frac{1}{2\pi} \sqrt{\frac{\pi}{Dt}} e^{-x^2/4Dt} \quad \left(\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}\right)$$
(187)

Hence the final result

$$\theta(x,t) = \frac{1}{2\sqrt{\pi Dt}} e^{-x^2/4Dt}$$
(188)

4.4 Laplace Transforms

Laplace transforms is useful for initial value problem where f(t) only exists for $t \geq 0$.

$$\mathcal{L}[f(t)] = \hat{f}(s) = \int_0^\infty dt e^{-st} f(t)$$
(189)

where s is a complex variable and $\mathrm{Re}(S)>0$ is required for the convergence of the integral.

4.4.1 Properties

• $\mathcal{L}[f'(t)] = s\hat{f}(s) - f(0)$ Proof.

$$\mathcal{L}[f'(t)] = \int_0^\infty dt e^{-st} f'(t)$$

$$= e^{-st} f(t) \Big|_0^\infty + s \int_0 dt e^{-st} f(t) = s \hat{f}(s) - f(0)$$
(190)

- $\mathcal{L}[f^{(n)}(t)] = s^n \hat{f}(s) s^{n-1} f(0) s^{n-2} f'(0) \dots f^{(n-1)}(0)$
- $\mathcal{L}[t^n f(t)] = (-1)^n \frac{\mathrm{d}^n}{\mathrm{d}s^n} \hat{f}(s)$

$$(-1)^{n} \frac{\mathrm{d}^{n}}{\mathrm{d}s^{n}} \hat{f}(s) = (-1)^{n} \frac{\mathrm{d}^{n}}{\mathrm{d}s^{n}} \int_{0}^{\infty} \mathrm{d}t \mathrm{e}^{-st} f(t)$$

$$= (-1)^{n} \int_{0}^{\infty} \mathrm{d}t (-t)^{n} \mathrm{e}^{-st} f(t)$$

$$= \int_{0}^{\infty} \mathrm{d}t \mathrm{e}^{-st} t^{n} f(t) = \mathcal{L}[t^{n} f(t)]$$

$$(191)$$

4.4.2 Examples

- $\mathcal{L}[1] = \frac{1}{s}$
- $\mathcal{L}[e^{-at}] = \frac{1}{s+a}$
- $\mathcal{L}[\cos \omega t] = \frac{s}{s^2 + w^2}$
- $\mathcal{L}[\sin \omega t] = \frac{w}{s^2 + w^2}$
- $\mathcal{L}[t^n] = \frac{n!}{s^{n+1}}$
- $\mathcal{L}[te^{-at}] = \frac{1}{(s+a)^2}$
- $\mathcal{L}[e^{at}f(t)] = \hat{f}(s-a)$

4.4.3 Convolution Theorem for Laplace Transforms

A convolution of two functions $f_1(t)$ and $f_2(t)$ is defined as

$$f_1 * f_2 = \int_{-\infty}^{\infty} f_1(t') f_2(t - t') dt'$$
 (192)

If f_1 and f_2 vanish for t < 0, then

$$f_1 * f_2 = \int_0^t f_1(t') f_2(t - t') dt'$$
(193)

If we apply the Laplace transform

$$\mathcal{L}[f_1 * f_2] = \int_0^\infty dt e^{-st} \int_0^t f_1(t') f_2(t - t') dt'$$

$$= \int_0^\infty dt' f_1(t') \int_{t'}^\infty dt e^{-st} f_2(t - t')$$

$$= \int_0^\infty dt' e^{-st'} f_1(t') \int_{t'}^\infty dt e^{-s(t - t')} f_2(t - t')$$

$$= \tilde{f}_1(s) \tilde{f}_2(s)$$
(194)

Example. Consider the differential equation

$$f'' + 5f' + 6f = 0 ag{195}$$

with boundary conditions f'(0) = f(0) = 0. Apply the Laplace transform on the equation, we have

$$s^{2}\hat{f} - sf(0) - f'(0) + 5[s\hat{f} - f(0)] + 6\hat{f} = \hat{f}(s^{2} + 5s + 6) = \frac{1}{s}$$
 (196)

rearranging this, we have

$$\hat{f}(s) = \frac{1}{s(s+2)(s+3)} = \frac{1}{6s} - \frac{1}{2}\frac{1}{s+2} + \frac{1}{3}\frac{1}{s+3}$$
 (197)

So

$$f(t) = \frac{1}{6} - \frac{1}{2}e^{-2t} + \frac{1}{3}e^{-3t}$$
 (198)