Imperial College London

NOTES

IMPERIAL COLLEGE LONDON

DEPARTMENT OF COMPUTING

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 $\{u_1, u_2, \cdots, u_n\}$ 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. $\langle \underline{v}, \underline{v} \rangle \geq 0$
4. Define $\|\underline{v}\| = \sqrt{\langle \underline{v}, \underline{v} \rangle}$. Then $\|\underline{v}\| = \underline{0} \;\Rightarrow\; \underline{v} = \underline{0}$

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. $\langle \underline{u}, \underline{v} \rangle = \langle \underline{v}, \underline{u} \rangle^*$
2. $\langle \underline{u}, a\underline{v}_1 + b\underline{v}_2 \rangle = a\langle \underline{u}, \underline{v}_1 \rangle + b\langle \underline{u}, \underline{v}_2 \rangle$
   $\langle a\underline{u}_1 + b\underline{u}_2, v \rangle = a^*\langle \underline{v}, \underline{u}_1 \rangle^* + b^*\langle \underline{v}, \underline{u}_2 \rangle^* = a^*\langle \underline{u}_1, \underline{v} \rangle + b^*\langle \underline{u}_2, \underline{v} \rangle$
3. $\langle \underline{v}, \underline{v} \rangle \geq 0$
4. Define $\|\underline{v}\| = \sqrt{\langle \underline{v}, \underline{v} \rangle}$. Then $\|\underline{v}\| = 0 \;\Rightarrow\; \underline{v} = \underline{0}$

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

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

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**.

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

- **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

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

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

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

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

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

A useful identity involving the contraction of two alternating tensors is

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

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

Proof 1

$$\begin{aligned} [\boldsymbol{a} \times (\boldsymbol{b} \times \boldsymbol{c})]_i &= \varepsilon_{ijk} a_j (\boldsymbol{b} \times \boldsymbol{c})_k \\ &= \varepsilon_{ijk} a_j \varepsilon_{klm} b_l c_m \\ &= (\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}) a_j b_l c_m \\ &= (a_j c_j) b_i - (a_j b_j) c_i \\ &= (\boldsymbol{a} \cdot \boldsymbol{c})[\boldsymbol{b}]_i - (\boldsymbol{a} \cdot \boldsymbol{b})[\boldsymbol{c}]_i \end{aligned} \tag{10}$$

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

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

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.

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

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 $\det(L) = 1$

$$x'_i = L_{ij} x_j \tag{14}$$

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

1.4.2 Transformation of Rank-Two Tensors

A rank-two tensor transforms as

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

For higher rank tensor,

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

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:

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

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

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

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

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

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

$$y(x) = ay_1(x) + by_2(x) \tag{22}$$

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

$$y(x) = ay_1(x) + by_2(x) + y_0(x) \tag{23}$$

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

$$y_0(x) = u(x)y_1(x) + v(x)y_2(x) \tag{24}$$

and the differential

$$y_0' = u'y_1 + uy_1' + v'y_2 + vy_2' \tag{25}$$

$$y_0'' = u''y_1 + 2u'y_1' + uy_1'' + v''y_2 + 2v'y_2' + vy_2'' \tag{26}$$

Substituting these expressions into the eqn.(21)

$$\begin{aligned}
\mathcal{L}_x[y_0(x)] =& u''y_1 + 2u'y_1' + uy_1'' + v''y_2 + 2v'y_2' + vy_2'' \\
& + p(u'y_1 + uy_1' + v'y_2 + vy_2') + q(uy_1 + vy_2) \\
=& u(y_1'' + py_1' + qy_1) + v(y_2'' + py_2' + qy_2) \\
& + u''y_1 + 2u'y_1' + v''y_2 + 2v'y_2' + p(u'y_1 + v'y_2) \\
=& u''y_1 + 2u'y_1' + v''y_2 + 2v'y_2' + p(u'y_1 + v'y_2)
\end{aligned} \tag{27}$$

Therefore, we will vary these parameters subject to the constraint

$$\boxed{u'y_1 + v'y_2 = 0} \tag{28}$$

and

$$u''y_1 + u'y_1' + v''y_2 + v'y_2' = 0 \tag{29}$$

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

$$\boxed{u'y_1' + v'y_2' = f} \tag{30}$$

So we have

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

then

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

where $W(x)$ is the *Wronskian*, and

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

So the solutions are

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

2.2.1 Homogeneous Initial Conditions

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

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

then

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

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

$$\begin{aligned} y(x) &= \int_\alpha^x \mathrm{d}\tilde{x} \frac{y_1(\tilde{x}) y_2(x) - y_2(\tilde{x}) y_1(x)}{W(\tilde{x})} f(\tilde{x}) + \int_x^\beta \mathrm{d}\tilde{x} \cdot 0 \\ &= \int_\alpha^\beta G(x, \tilde{x}) f(\tilde{x}) \mathrm{d}\tilde{x} \end{aligned} \tag{37}$$

where we have defined the *Green Function*

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

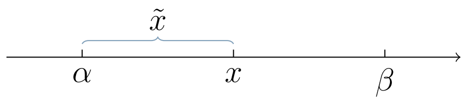

Figure 1: The range of variable x in the problem is $x \in [\alpha, \beta]$.

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

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

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

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

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

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

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

$$\begin{aligned} y(\beta) &= y_0(\beta) + ay_1(\beta) + by_2(\beta) \\ &= -\int_\alpha^\beta \mathrm{d}\tilde{x} \frac{y_1(\beta)y_2(\tilde{x})}{W(\tilde{x})} f(\tilde{x}) + ay_1(\beta) = 0 \quad \Rightarrow \quad a = \int_\alpha^\beta \mathrm{d}\tilde{x} \frac{y_2(\tilde{x})}{W(\tilde{x})} f(\tilde{x}) \end{aligned} \tag{43}$$

which may be substituted in to the solution to give

$$\begin{aligned} y(x) &= \int_\alpha^x \mathrm{d}\tilde{x} \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) + ay_1(x) \\ &= \int_\alpha^x \mathrm{d}\tilde{x} \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) + \int_\alpha^\beta \mathrm{d}\tilde{x} \frac{y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) \\ &= \int_\alpha^x \mathrm{d}x \frac{y_1(\tilde{x})y_2(x)}{W(\tilde{x})} f(\tilde{x}) + \int_x^\beta \mathrm{d}x \frac{y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) \\ &= \int_\alpha^\beta \mathrm{d}\tilde{x} G(x, \tilde{x}) f(\tilde{x}) \end{aligned} \tag{44}$$

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 $x = \tilde{x}$
$$\begin{aligned}\lim_{\varepsilon\to 0}\left[\frac{\partial G(x,\tilde{x})}{\partial x}\right]_{x=\tilde{x}-\varepsilon}^{x=\tilde{x}+\varepsilon} &= \lim_{\varepsilon\to 0}\left[\frac{y_1(\tilde{x})y_2'(\tilde{x}+\varepsilon)}{W(\tilde{x})} - \frac{y_2(\tilde{x})y_1'(\tilde{x}-\varepsilon)}{W(\tilde{x})}\right] \\ &= \frac{W(\tilde{x})}{W(\tilde{x})} = 1\end{aligned} \tag{48}$$

2.3 Green Function More Generally

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

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

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

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

$G(x,\tilde{x})$ 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

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

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.

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

$f(x)$ 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

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

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

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

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 $y_2(x)$
$$G(x, \tilde{x}) = A(\tilde{x}) y_1(x) + B(\tilde{x}) y_2(x) \tag{55}$$
We can find A and B by using the properties of G:

   (i) G is continuous at $x = \tilde{x}$
$$A(\tilde{x}) y_1(\tilde{x}) + B(\tilde{x}) y_2(\tilde{x}) = 0 \tag{56}$$

   (ii) G' has a unit discontinuity at $x = \tilde{x}$
$$A(\tilde{x}) y_1'(\tilde{x}) + B(\tilde{x}) y_2'(\tilde{x}) = 0 \tag{57}$$

   The solution is
$$A(\tilde{x}) = -\frac{y_x(\tilde{x})}{W(\tilde{x})}, \qquad B(\tilde{x}) = \frac{y_1(\tilde{x})}{W(\tilde{x})} \tag{58}$$
where W is the Wronskian of y_1 and y_2.

So we have
$$G(x, \tilde{x}) = \begin{cases} 0, & x < \tilde{x} \\ \frac{y_1(\tilde{x}) y_2(x) - y_2(\tilde{x}) y_1(x)}{W(\tilde{x})}, & x > \tilde{x} \end{cases} \tag{59}$$
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 $y_1(\alpha) = y_2(\beta) = 0$.

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

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

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

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

   so we have

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

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

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

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

   so we have

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

The final result

$$G(x, \tilde{x}) = \begin{cases} \frac{y_2(\tilde{x})y_1(x)}{W(\tilde{x})}, & \alpha < x < \tilde{x} \\ \frac{y_1(\tilde{x})y_2(x)}{W(\tilde{x})}, & \tilde{x} < x < \beta \end{cases} \tag{68}$$

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

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

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

$$\int_R \mathrm{d}\tilde{x}_1 \mathrm{d}\tilde{x}_2 \delta^{(2)}(\underline{x} - \underline{\tilde{x}}) f(\underline{\tilde{x}}) = \begin{cases} f(\underline{x}), & \underline{x} \in R \\ 0 & \underline{x} \notin R \end{cases} \tag{71}$$

Example. The most famous example is

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

and the Green function satisfies

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

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

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

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

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

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

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
$$\langle f, g \rangle = \int_a^b f^*(x) g(x) \mathrm{d}x \tag{77}$$
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 $\{y_1, y_2, y_3, \cdots\}$ is orthogonal.

2. Let $\{y_1, y_2, y_3, \cdots\}$ be an orthogonal basis, then any function $f(x) \in \mathcal{H}$ can be expanded
$$f(x) = \sum_{i=1}^{\infty} f_i y_i(x), \quad f_i \in \mathbb{C} \tag{78}$$
Then we have
$$\langle y_k, f \rangle = \langle y_k, \sum_{i=1}^{\infty} f_i y_i \rangle = \sum_{i=1}^{\infty} f_i \langle y_k, y_i \rangle = \sum_{i=1}^{\infty} f_i \delta_{ik} = f_k \tag{79}$$

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
$$\boxed{\mathcal{L} = -\frac{\mathrm{d}}{\mathrm{d}x}\left[\rho(x)\frac{\mathrm{d}}{\mathrm{d}x}\right] + \sigma(x)} \tag{80}$$
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
$$\boxed{\langle u, \mathcal{D}v \rangle = \langle v, \mathcal{D}u \rangle^*, \quad \forall u, v \in \mathcal{H}} \tag{82}$$

[1]being 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 $M : M_{ij} = M^*_{ji}$.

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

$$\begin{aligned}
\langle u, \mathcal{L}v\rangle &= \int_a^b u^* \left[-(\rho v')' + \sigma v\right] \mathrm{d}x \\
&= - u^*\rho v'\big|_a^b + \int_a^b \left(u^{*\prime}\rho v' + u^*\sigma v\right) \mathrm{d}x \\
&= - u^*\rho v'\big|_a^b + u^{*\prime}\rho v\big|_a^b + \int_a^b \left(-(u^{*\prime}\rho)' v + u^*\sigma v\right) \mathrm{d}x \\
&= (-u^*\rho v' + u^{*\prime}\rho v)\big|_a^b + \int_a^b \left(-(u^{*\prime}\rho)' + u^*\sigma\right) v \mathrm{d}x \\
&= (-u^*\rho v' + u^{*\prime}\rho v)\big|_a^b + \left[\int_a^b \left(-(u'\rho)' + u\sigma\right) v^* \mathrm{d}x\right]^* \\
&= (-u^*\rho v' + u^{*\prime}\rho v)\big|_a^b + \langle v, \mathcal{L}u\rangle^*
\end{aligned} \tag{83}$$

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

$$\rho(u^{*\prime}v - u^*v')\big|_a^b = 0 \tag{84}$$

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

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

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

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

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.*

$$w(x)\left[-(Ay')' - By' + Cy\right] = -(\rho y')' + \sigma y \tag{87}$$

rearranging this

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

so we have

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

then

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

We choose w(x) such that

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

where $w(a) = 1$.

Definition. The inner product with weight w

$$\langle f, g\rangle_w = \langle f, wg\rangle = \int_a^b f^*(x)w(x)g(x)\mathrm{d}x = \langle wf, g\rangle \tag{92}$$

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

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

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

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

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

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

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

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

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

- 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

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

where

$$g_n = \langle f_n, g\rangle_w = \int_a^b f_n^*(x) w(x) g(x) \mathrm{d}x \tag{105}$$

Substituting into the expansion we find

$$\begin{aligned} g(x) &= \sum_n \int_a^b \mathrm{d}\tilde{x}\,[f_n^*(\tilde{x}) w(\tilde{x}) g(\tilde{x})]\, f_n(x) \\ &= \int_a^b \mathrm{d}\tilde{x} g(\tilde{x}) \left[w(\tilde{x}) \sum_n f_n(x) f_n^*(\tilde{x})\right] \\ &= \int_a^b \mathrm{d}\tilde{x} \delta(x - \tilde{x}) g(\tilde{x}) \end{aligned} \tag{106}$$

where

$$\boxed{\delta(x - \tilde{x}) = w(\tilde{x}) \sum_n f_n(\tilde{x}) f_n^*(\tilde{x})} \tag{107}$$

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

$$\begin{aligned}\int_a^b |u|^2 \omega \mathrm{d}x =& \langle u, u\rangle_w = \langle \sum_n u_n f_n(x), \sum_m u_m f_m(x)\rangle_w \\ =& \sum_{n,m} u_n^* u_m \langle f_n, f_m\rangle_w = \sum_{n,m} u_n^* u_m \delta_{nm} = \sum_n |u_n|^2\end{aligned} \tag{108}$$

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

$$\boxed{G(x, \tilde{x}) = \sum_n \frac{y_n(x) y_n^*(\tilde{x})}{\lambda_n}} \tag{110}$$

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

$$\begin{aligned}\mathcal{L}_x[G(x,\tilde{x})] =& \sum_n \frac{\mathcal{L}_x[y_n(x)] y_n^*(\tilde{x})}{\lambda_n} \\ =& \sum_n w(x) y_n(x) y_n^*(\tilde{x}) \\ =& \frac{\omega(x)}{\omega(\tilde{x})}\left[\omega(\tilde{x}) \sum_n y_n(x) y_n^*(\tilde{x})\right] \\ =& \delta(x - \tilde{x}) \quad \square\end{aligned} \tag{111}$$

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

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

Substituting into the original equation, we find

$$\begin{aligned} & \mathcal{L}\sum_n a_n y_n - \nu \sum_n a_n y_n = \sum_n f_n y_n \\ \Rightarrow \quad & \sum_n (a_n \lambda_n - \nu a_n) y_n = \sum_n f_n y_n \\ \Rightarrow \quad & (a_n \lambda_n - \nu a_n) = f_n\end{aligned} \tag{114}$$

So that

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

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

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

Example. Let

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

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

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

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