

NOTES

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DEPARTMENT OF PHYSICS

Mathematical Methods for Physicists

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Merry Christmas :D

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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 $-\underline{u}$ such that: $\underline{u} + (-\underline{u}) = \underline{0}$.
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

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

2 component complex vectors

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

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 $\{u_1, u_2, \dots, u_n\}$ 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 $\|\underline{v}\| = 0 \Rightarrow \underline{v} = \underline{0}$

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. $\langle \underline{u}, a\underline{v}_1 + b\underline{v}_2 \rangle = a\langle \underline{u}, \underline{v}_1 \rangle + b\langle \underline{u}, \underline{v}_2 \rangle$
 $\langle a\underline{u}_1 + b\underline{u}_2, \underline{v} \rangle = a^*\langle \underline{v}, \underline{u}_1 \rangle^* + b^*\langle \underline{v}, \underline{u}_2 \rangle^* = a^*\langle \underline{u}_1, \underline{v} \rangle + b^*\langle \underline{u}_2, \underline{v} \rangle$
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.

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

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 $\{\underline{e}_1, \dots, \underline{e}_n\}$ 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 m rows and n columns.

1.2.1 Summation Convention

The expression for the elements of $C = AB$ is

$$C_{ij} = \sum_k A_{ik} B_{kj} \quad (3)$$

and this may be written as

$$C_{ij} = A_{ik} B_{kj} \quad (4)$$

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.**

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

- **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

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

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

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

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

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

A useful identity involving the contraction of two alternating tensors is

$$\varepsilon_{ijk} \varepsilon_{klm} = \delta_{il} \delta_{jm} - \delta_{im} \delta_{jl} \quad (9)$$

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

Proof.

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

1.2.4 Eigenvalues, Eigenvectors and Diagonalization

An eigenvalue equation takes the form

$$A_{ij} x_j = \lambda x_i \quad (11)$$

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 $\{e^{(1)}, \dots, e^{(n)}\}$. Then M is an orthogonal matrix and

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

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.

$$J_i = \sigma_{ij} E_j \quad (13)$$

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 $\det(L) = 1$

$$x'_i = L_{ij}x_j \quad (14)$$

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

1.4.2 Transformation of Rank-Two Tensors

A rank-two tensor transforms as

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

For higher rank tensor,

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

1.5 Tensor Calculus

1.5.1 The Gradient Operator

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

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

$$[\nabla\phi]_i = \partial_i\phi \quad (18)$$

$$\nabla \cdot \mathbf{F} = \partial_i F_i \quad (19)$$

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

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

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

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

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

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

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

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

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

and the differential

$$y'_0 = u'y_1 + uy'_1 + v'y_2 + vy'_2 \quad (25)$$

$$y''_0 = u''y_1 + 2u'y'_1 + uy''_1 + v''y_2 + 2v'y'_2 + vy''_2 \quad (26)$$

Substituting these expressions into the eqn.(21)

$$\begin{aligned} \mathcal{L}_x[y_0(x)] &= u''y_1 + 2u'y'_1 + uy''_1 + v''y_2 + 2v'y'_2 + vy''_2 \\ &\quad + p(u'y_1 + uy'_1 + v'y_2 + vy'_2) + q(uy_1 + vy_2) \\ &= u(y''_1 + py'_1 + qy_1) + v(y''_2 + py'_2 + qy_2) \\ &\quad + u''y_1 + 2u'y'_1 + v''y_2 + 2v'y'_2 + p(u'y_1 + v'y_2) \\ &= u''y_1 + 2u'y'_1 + v''y_2 + 2v'y'_2 + p(u'y_1 + v'y_2) \end{aligned} \quad (27)$$

Therefore, we will vary these parameters subject to the constraint

$$\boxed{u'y_1 + v'y_2 = 0} \quad (28)$$

and

$$u''y_1 + u'y'_1 + v''y_2 + v'y'_2 = 0 \quad (29)$$

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

$$\boxed{u'y'_1 + v'y'_2 = f} \quad (30)$$

So we have

$$\begin{cases} u'y'_1 + v'y'_2 = f \\ u'y_1 + v'y_2 = 0 \end{cases} \Rightarrow \begin{pmatrix} y_1 & y_2 \\ y'_1 & y'_2 \end{pmatrix} \begin{pmatrix} u' \\ v' \end{pmatrix} = M \begin{pmatrix} u' \\ v' \end{pmatrix} = \begin{pmatrix} 0 \\ f \end{pmatrix} \quad (31)$$

then

$$\begin{pmatrix} u' \\ v' \end{pmatrix} = M^{-1} \begin{pmatrix} 0 \\ f \end{pmatrix} = \frac{1}{W(x)} \begin{pmatrix} y'_2 & -y_2 \\ -y'_1 & y_1 \end{pmatrix} \begin{pmatrix} 0 \\ f \end{pmatrix} \quad (32)$$

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

$$W(x) = \det(M) = y_1y'_2 - y_2y'_1 \quad (33)$$

So the solutions are

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

2.2.1 Homogeneous Initial Conditions

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

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

then

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

satisfies $y_0(\alpha) = y'_0(\alpha) = 0$. So $y = y_0$ is a solution of the ODE with boundary conditions $y(\alpha) = y'(\alpha) = 0$.

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

where we have defined the *Green Function*

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

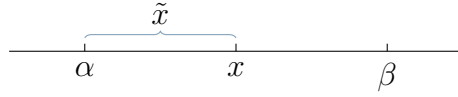


Figure 1: The range of variable x in the problem is $x \in [\alpha, \beta]$.

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

$$Y(x) = y(x) - g(x) \quad (39)$$

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

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

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

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

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

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

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

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

which may be substituted in to the solution to give

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

where we have defined the *Green Function*

$$G(x, \tilde{x}) = \begin{cases} \frac{y_1(\tilde{x})y_2(x)}{W(\tilde{x})}, & \alpha \leq \tilde{x} < x \\ \frac{y_2(\tilde{x})y_1(x)}{W(\tilde{x})}, & x < \tilde{x} \leq \beta \end{cases} \quad (45)$$

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 $x \neq \tilde{x}$

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

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

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

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

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

2.3 Green Function More Generally

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

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

$\delta(x)$ 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

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

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.

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

$f(x)$ 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

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

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

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

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 $x < \tilde{x}$

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

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 $y_2(x)$

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

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

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

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

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

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

The solution is

$$A(\tilde{x}) = -\frac{y_2(\tilde{x})}{W(\tilde{x})}, \quad B(\tilde{x}) = \frac{y_1(\tilde{x})}{W(\tilde{x})} \quad (58)$$

where W is the Wronskian of y_1 and y_2 .

So we have

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

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

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

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

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

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

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

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

so we have

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

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

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

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

so we have

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

The final result

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

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

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

and

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

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

$$\int_R d\tilde{x}_1 d\tilde{x}_2 d\tilde{x}_3 \delta^{(2)}(\underline{x} - \underline{\tilde{x}}) f(\underline{\tilde{x}}) = \begin{cases} f(\underline{x}), & \underline{x} \in R \\ 0 & \underline{x} \notin R \end{cases} \quad (71)$$

Example. The most famous example is

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

and the Green function satisfies

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

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

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

and

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

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

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

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 $\{u_1, u_2, u_3, \dots\}$. 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

$$\langle f, g \rangle = \int_a^b f^*(x)g(x)dx \quad (77)$$

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

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

Then we have

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

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

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

and

$$\mathcal{L}y = -\frac{d}{dx} \left(\rho \frac{dy}{dx} \right) + \sigma y = -(\rho y')' + \sigma y \quad (81)$$

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

$$\boxed{\langle u, \mathcal{D}v \rangle = \langle v, \mathcal{D}u \rangle^*, \quad \forall u, v \in \mathcal{H}} \quad (82)$$

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 $M : M_{ij} = M_{ji}^*$.

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

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

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

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

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

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

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.

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

rearranging this

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

so we have

$$\begin{cases} -(Aw y')' + w' A y' - B w y' = -(\rho y')' \\ C w y = \sigma y \end{cases} \quad (89)$$

then

$$\frac{w'}{w} = \frac{B}{A}, \quad Aw = \rho, \quad Cw = \sigma \quad (90)$$

We choose $w(x)$ such that

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

where $w(a) = 1$.

Definition. The inner product with weight w

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

w is real.

3.1.4 Eigenfunctions and Eigenvalues

Consider the inhomogeneous eigenfunction equation

$$\tilde{\mathcal{L}}y = \lambda y \quad (93)$$

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

$$\boxed{\mathcal{L}y = \lambda wy} \quad (94)$$

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

$$\mathcal{L}y_i = \lambda_i wy_i \quad (95)$$

$$\langle y_j, \mathcal{L}y_i \rangle = \lambda_i \langle y_j, wy_i \rangle \quad (96)$$

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

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

$$\mathcal{L}y_j = \lambda_j w y_j \quad (99)$$

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

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

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

- For $i = j$ we have

$$(\lambda_i^* - \lambda_i) \|y_i\|_w^2 = 0 \quad (102)$$

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

- For $i \neq j$ we have

$$(\lambda_i - \lambda_j) \langle y_i, y_j \rangle_w = 0 \quad (103)$$

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 $\lambda_1, \lambda_2, \lambda_3, \dots$ such that $|\lambda_n| \rightarrow \infty$ as $n \rightarrow \infty$, and that the corresponding eigenfunctions with weight w , f_1, f_2, f_3, \dots 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

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

where

$$g_n = \langle f_n, g \rangle_w = \int_a^b f_n^*(x) w(x) g(x) dx \quad (105)$$

Substituting into the expansion we find

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

where

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

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

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

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

$$\langle u, u \rangle_w = \sum_n |u_n|^2 \quad (109)$$

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

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

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

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

3.1.7 Eigenfunction Expansions for Solving ODEs

As an example, consider the differential equation

$$\mathcal{L}y - \nu y = f \quad (112)$$

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

$$y(x) = \sum_n a_n y_n(x), \quad f(x) = \sum_n f_n y_n(x) \quad (113)$$

Substituting into the original equation, we find

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

So that

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

so that the solution is given by

$$y(x) = \sum_n \frac{f_n}{\lambda_n - \nu} y_n(x) \quad (116)$$

3.2 Legendre Polynomials

3.2.1 Two Examples

Example. Let

$$\mathcal{L} = -\frac{d^2}{dx^2}, \quad x \in [0, 2\pi R] \quad (117)$$

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

$$-y_n'' = \lambda_n y_n \quad (118)$$

and the eigenfunctions and the corresponding eigenvalues are

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

Example. Let

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

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

$$-y_m'' = \lambda_m y_m \quad (121)$$

and the eigenfunctions and the corresponding eigenvalues are

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

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

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

Assume that eigenfunctions of eqn.(123) are polynomials

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

substituting this to the eigenfunction equation, we have

$$m_n(m_n + 1) = \lambda \quad (125)$$

So eigenvalues take form

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

We can label the eigenfunctions by l

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

$$\int_{-1}^1 y_l^*(x) y_{l'}(x) dx = \delta_{ll'} \quad (127)$$

3.2.2 Legendre's Equation

Legendre's equation

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

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 $\lambda = l(l + 1)$.

$$\boxed{-\frac{d}{dx} [(1-x^2)y'] = l(l+1)y} \quad (129)$$

or

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

where

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

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

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

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

$$m_n(m_n + 1) = \lambda \quad (133)$$

So eigenvalues take form

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

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

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

If we take

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

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

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

Rearrange this, we have

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

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

$$\frac{d}{d\theta} = \frac{d}{du} \frac{du}{d\theta} = -\sin \theta \frac{d}{du} \quad (139)$$

Then the equation becomes

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

self-adjoint form

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

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

Similarly, the equation can be expressed as

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

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

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

Finally we get

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

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

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

So any function f can be expressed as

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

where

$$f_{lm} = \int_{\mathbb{S}^2} Y_l^{m*} f d\Omega \quad (147)$$

4 Integral Transforms

4.1 Fourier Series

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

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

where

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

and we have

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

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

$$\begin{aligned} f_n &= \int_{-\pi R}^{\pi R} y_n^*(x) f(x) dx \\ &= \frac{1}{\sqrt{2\pi R}} \int_{-\pi R}^{\pi R} e^{-inx/R} f(x) dx \\ &= \frac{1}{\sqrt{2\pi R}} \int_{-\pi R}^{\pi R} e^{-ik_n x} f(x) dx \end{aligned} \quad (151)$$

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

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

for f satisfying $\int_{-\infty}^{\infty} |f| dx$ 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

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

The *inverse Fourier transform* is defined as

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

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

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

4.2.2 Dirac Delta-Function

$$\begin{aligned}
f(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx} dk \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x') e^{-ikx'} dx' \right] e^{ikx} dk \\
&= \int_{-\infty}^{\infty} f(x') \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-x')} dk \right] dx' \\
&= \int_{-\infty}^{\infty} f(x') \delta(x - x') dx'
\end{aligned} \tag{156}$$

where we have defined the *Dirac delta-function*

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

4.2.3 Properties of the Fourier Transform

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

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

- 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

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

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

Proof. Define $y = -x$, then

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

2. Differentiation

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

Proof. Consider the first order derivative

$$\begin{aligned}
\text{TF}[f'(x)] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-ikx} f'(x) \\
&= \frac{1}{\sqrt{2\pi}} [f(x) e^{-ikx}]_{-\infty}^{\infty} - \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx f(x) (-ik) e^{-ikx} \\
&= ik \tilde{f}(k)
\end{aligned} \tag{162}$$

3. Multiplication by x

$$\text{FT}[xf(x)] = i \frac{d}{dk} \tilde{f}(k) \quad (163)$$

4. Rigid shift of coordinate

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

Proof. Define $y = x - a$, then

$$\begin{aligned} \text{FT}[f(x - a)] &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} f(x - a) dx \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ika} e^{-ik(x-a)} f(x - a) d(x - a) \\ &= \frac{1}{\sqrt{2\pi}} e^{-ika} \int_{-\infty}^{\infty} e^{-iky} f(y) dy = e^{-ika} \tilde{f}(k) \end{aligned} \quad (165)$$

4.2.4 Parseval's Theorem

Parseval's theorem for Fourier transforms states that

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

Proof.

$$\begin{aligned} \int_{-\infty}^{\infty} |f(x)|^2 dx &= \int_{-\infty}^{\infty} f(x) f^*(x) dx \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \tilde{f}(k) \tilde{f}^*(k') e^{i(k-k')x} \right] dx \\ &= \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \tilde{f}(k) \tilde{f}^*(k') \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i(k-k')x} dx \right] \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \tilde{f}(k) \tilde{f}^*(k') \delta(k - k') dk dk' \\ &= \int_{-\infty}^{\infty} \tilde{f}(k) \tilde{f}^*(k) dk = \int_{-\infty}^{\infty} |\tilde{f}(k)|^2 dk \end{aligned} \quad (167)$$

4.2.5 Convolution Theorem

The convolution of f and g is defined as

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

with claims

1. $f * g = g * f$

2. $f * \delta = f$

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

1.

$$\begin{aligned} \text{FT}(f * g) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-ikx} \int_{-\infty}^{\infty} dy f(y) g(x-y) \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dy e^{-iky} f(y) \int_{-\infty}^{\infty} dx e^{-ik(x-y)} g(x-y) \\ &= \sqrt{2\pi} \tilde{f}(k) \tilde{g}(k) = \sqrt{2\pi} \text{FT}[f] \text{FT}[g] \end{aligned} \quad (169)$$

2.

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

4.2.6 Examples of Fourier Transform

1. Constant function $f(x) = 1$

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

2. Single frequency/wavenumber mode $f(x) = e^{ik_0 x}$

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

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

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

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

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

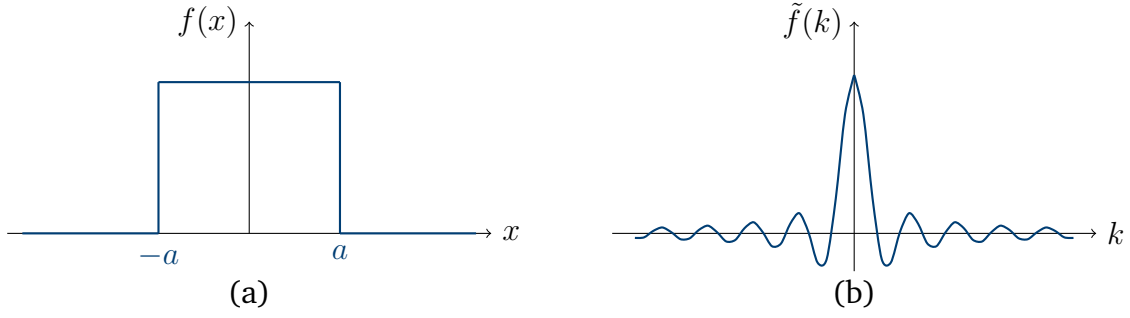


Figure 2: Top-hat function.

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

$$\begin{aligned} \tilde{f}(k) &= \frac{1}{\sqrt{2\pi}} \int_{-a}^a e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \left[-\frac{1}{ik} e^{-ikx} \right]_{-a}^a \\ &= \sqrt{\frac{2}{\pi}} \frac{\sin(ka)}{k} = a \sqrt{\frac{2}{\pi}} \text{sinc}(ak) \end{aligned} \quad (175)$$

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

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

so we have

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

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

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

4.3.2 Double Slit Diffraction

The aperture function is given by

$$h(x) = f(x)g(x) \quad (179)$$

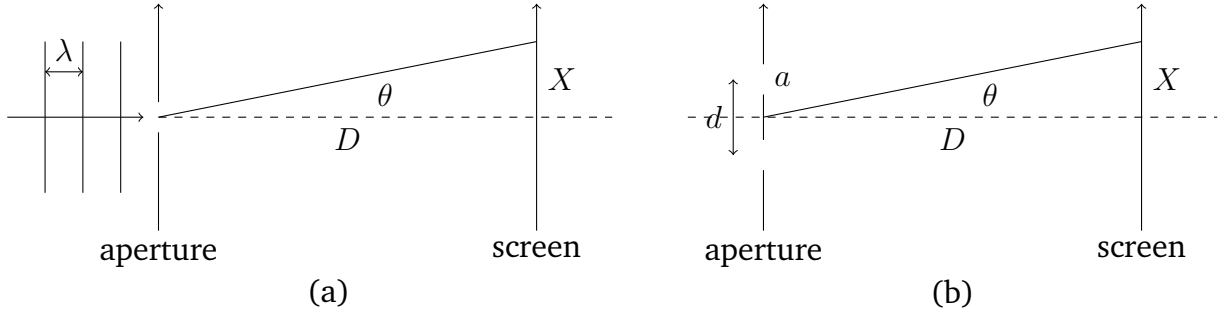


Figure 3: Geometry for Fraunhofer diffraction. (a) Diffraction through an aperture. (b) Double slit diffraction.

where

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

and $g(x)$ is single aperture function. And

$$\begin{aligned} \tilde{f}(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-ikx} \left[\delta\left(x - \frac{d}{2}\right) + \delta\left(x + \frac{d}{2}\right) \right] \\ &= \frac{1}{\sqrt{2\pi}} (e^{-ikd/2} + e^{ikd/2}) = \sqrt{\frac{2}{\pi}} \cos\left(\frac{kd}{2}\right) \end{aligned} \quad (181)$$

so we have

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

and the intensity on the screen is given by

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

4.3.3 Diffusion Equation

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

$$\frac{\partial \theta}{\partial t} = D \frac{\partial^2 \theta}{\partial x^2} \quad (184)$$

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

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

the solution is

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

So we have

$$\begin{aligned} \theta(x, t) &= \text{FT}^{-1}[\tilde{\theta}(k, t)] \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ikx} e^{-Dk^2t} \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \exp \left[-Dt \left(k - \frac{ix}{2Dt} \right)^2 - \frac{x^2}{4Dt} \right] dk \\ &= \frac{1}{2\pi} e^{-x^2/4Dt} \int_{-\infty}^{\infty} e^{-Dtq^2} dq \\ &= \frac{1}{2\pi} \sqrt{\frac{\pi}{Dt}} e^{-x^2/4Dt} \left(\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}} \right) \end{aligned} \quad (187)$$

Hence the final result

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

4.4 Laplace Transforms

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

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

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

4.4.1 Properties

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

Proof.

$$\begin{aligned} \mathcal{L}[f'(t)] &= \int_0^{\infty} dt e^{-st} f'(t) \\ &= e^{-st} f(t) \Big|_0^{\infty} + s \int_0^{\infty} dt e^{-st} f(t) = s\hat{f}(s) - f(0) \end{aligned} \quad (190)$$

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

Proof.

$$\begin{aligned} (-1)^n \frac{d^n}{ds^n} \hat{f}(s) &= (-1)^n \frac{d^n}{ds^n} \int_0^{\infty} dt e^{-st} f(t) \\ &= (-1)^n \int_0^{\infty} dt (-t)^n e^{-st} f(t) \\ &= \int_0^{\infty} dt e^{-st} t^n f(t) = \mathcal{L}[t^n f(t)] \end{aligned} \quad (191)$$

4.4.2 Examples

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

4.4.3 Convolution Theorem for Laplace Transforms

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

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

If f_1 and f_2 vanish for $t < 0$, then

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

If we apply the Laplace transform

$$\begin{aligned} \mathcal{L}[f_1 * f_2] &= \int_0^{\infty} dt e^{-st} \int_0^t f_1(t')f_2(t-t')dt' \\ &= \int_0^{\infty} dt' f_1(t') \int_{t'}^{\infty} dt e^{-st} f_2(t-t') \\ &= \int_0^{\infty} dt' e^{-st'} f_1(t') \int_{t'}^{\infty} dt e^{-s(t-t')} f_2(t-t') \\ &= \tilde{f}_1(s)\tilde{f}_2(s) \end{aligned} \quad (194)$$

Example. Consider the differential equation

$$f'' + 5f' + 6f = 0 \quad (195)$$

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

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

rearranging this, we have

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

So

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

5 Complex Analysis

5.1 Complex Functions of a Complex Variable

A complex number $z = x + iy$ can be mapped to another complex number $w = f(z) = u(x, y) + iv(x, y)$. It is often useful to use the ‘polar representation’ of complex numbers where

$$z = re^{i\theta} \quad (199)$$

where $r = |z| = \sqrt{x^2 + y^2}$ is called the modulus of z and $\theta = \arg(z)$ is called the argument of z . $\arg(z)$ can be made unambiguous by a choice of ‘branch’. We will write the principal branch as $\text{Arg}(z)$, which is values $-\pi < \text{Arg}(z) \leq \pi$.

Example.

$$1) f(z) = |z| = \sqrt{x^2 + y^2}$$

$$2) f(z) = \frac{1}{z} = \frac{1}{x+iy} = \frac{x}{x^2+y^2} - i\frac{y}{x^2+y^2}$$

$$3) f(z) = z^3 = (x + iy)^3 = (x^3 - 3xy^2) + i(3x^2y - y^3)$$

$$4) f(z) = z^{1/3} = r^{1/3}e^{(i\theta+2\pi in)/3} = \begin{cases} r^{1/3} \exp\left(\frac{i\theta}{3}\right) \\ r^{1/3} \exp\left(\frac{i\theta}{3} + \frac{2\pi i}{3}\right) \\ r^{1/3} \exp\left(\frac{i\theta}{3} + \frac{4\pi i}{3}\right) \end{cases}$$

Complex functions defined as power series

$$e^z = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \dots \quad (200)$$

$$\cos z = 1 - \frac{z^2}{2!} + \frac{z^4}{4!} - \dots \quad (201)$$

$$\ln(1 + z) = z - \frac{z^2}{2} + \frac{z^3}{3} - \dots \quad (|z| < 1) \quad (202)$$

5.2 Continuity, Differentiability and Analyticity

5.2.1 Definitions

Definition. $f(z)$ is *continuous* at $z = z_0$ if $\forall \varepsilon > 0$, there exists a $\delta > 0$, such that, if $|z - z_0| < \delta$ then $|f(z) - f(z_0)| < \varepsilon$. We also say

$$\lim_{z \rightarrow z_0} f(z) = f(z_0) \quad (203)$$

Definition. $f(z)$ is *differentiable* at $z = z_0$ if $\exists F \in \mathbb{C}$ such that

$$\lim_{z \rightarrow z_0} \frac{f(z) - f(z_0)}{z - z_0} = F \quad (204)$$

we say $f'(z_0) = (df/dz)|_{z_0} = F$.

Definition. A subset $D \subset \mathbb{C}$ is *open* if for every $z \in D$, there is an open disc centred at z entirely contained in D .

Definition. A function $f(z)$ is *analytic* at z_0 if $f(z)$ is differentiable everywhere in an open domain containing z_0 ; if $f(z)$ is NOT analytic at z_0 we say $f(z)$ is *singular* at z_0 .

Example. $f(z) = z^2$ and $z = z_0 + \delta z$

$$\lim_{\delta z \rightarrow 0} \frac{(z_0 + \delta z)^2 - z_0^2}{\delta z} = 2z_0 \quad (205)$$

$f(z) = z^2$ is differentiable everywhere in \mathbb{C} . So we say $f(z)$ is analytic in \mathbb{C} and $f(z)$ is entire.

Example. $f(z) = z^* = x - iy$ and $z = z_0 + \delta z$

$$\lim_{\delta z \rightarrow 0} \frac{(z_0 + \delta z)^* - z_0^*}{\delta z} = \lim_{\delta z \rightarrow 0} \frac{\delta z^*}{\delta z} = e^{-2i\theta} \quad (206)$$

$f(z) = z^*$ is not differentiable anywhere so $f(z)$ is not analytic in \mathbb{C} .

5.2.2 The Cauchy-Riemann Conditions

In this section we ask: *Under what conditions is a complex function $f(z) = u(x, y) + iv(x, y)$ analytic in a domain D ?* Let us assume that $\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial v}{\partial x}, \frac{\partial v}{\partial y}$ all exist in D , i.e., $f(z)$ is analytic in D .

$$\frac{\partial f}{\partial x} = \frac{\partial z}{\partial x} \frac{df}{dz} = f', \quad \frac{\partial f}{\partial y} = \frac{\partial z}{\partial y} \frac{df}{dz} = if' \quad (207)$$

which shows

$$i \frac{\partial f}{\partial x} = \frac{\partial f}{\partial y} \Rightarrow i \left(\frac{\partial u}{\partial x} + i \frac{\partial v}{\partial x} \right) = \left(\frac{\partial u}{\partial y} + i \frac{\partial v}{\partial y} \right) \quad (208)$$

Rearranging this, now we get the *Cauchy-Riemann equations*

$$\boxed{\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}} \quad (209)$$

It is a theorem that $f(z)$ is analytic if and only if Cauchy-Riemann equations hold in D .

Example. $f(z) = z^2 = (x + iy)^2 = (x^2 - y^2) + 2ixy$. In this function, $u = x^2 - y^2$ and $v = 2xy$.

$$\frac{\partial u}{\partial x} = 2x, \quad \frac{\partial u}{\partial y} = -2y \quad (210)$$

$$\frac{\partial v}{\partial x} = 2y, \quad \frac{\partial v}{\partial y} = 2x \quad (211)$$

satisfy the C-R equations.

Example. $f(z) = x = (z + z^*)/2$. In this function, $u = x$ and $v = 0$, so we have

$$\frac{\partial u}{\partial x} = 1 \neq \frac{\partial v}{\partial y} = 0 \quad (212)$$

C-R equations fail.

Example. $f(z) = x^2 + y^2 = zz^*$ with $u = x^2 + y^2$ and $v = 0$.

$$\frac{\partial u}{\partial x} = 2x, \quad \frac{\partial u}{\partial y} = 2y, \quad \frac{\partial v}{\partial x} = \frac{\partial v}{\partial y} = 0 \quad (213)$$

So $f(z)$ satisfies C-R equations at $x = y = 0$ but nowhere else.

Theorem. $f(z)$ is analytic at $z = z_0$ if and only if $f(z)$ has a power series expansion around $z = z_0$ that converges in an open neighborhood of z_0 .

$$f(z) = c_0 + c_1(z - z_0) + c_2(z - z_0)^2 + \cdots = \sum_{k=0}^{\infty} c_k(z - z_0)^k \quad (214)$$

with

$$c_k = \frac{f^{(k)}(z_0)}{k!} \quad (215)$$

5.2.3 Harmonic Functions

Definition. $g(x, y)$ is harmonic if $\nabla^2 g = 0$.

Now we look at C-R equations

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial x} \frac{\partial u}{\partial x} = \frac{\partial}{\partial x} \frac{\partial v}{\partial y} = \frac{\partial}{\partial y} \frac{\partial v}{\partial x} = -\frac{\partial}{\partial y} \frac{\partial u}{\partial y} = -\frac{\partial^2 u}{\partial y^2} \quad (216)$$

Hence

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \nabla^2 u = 0 \quad (217)$$

$u(x, y)$ is harmonic. Similarly, $v(x, y)$ is harmonic. We conclude that if $f = u + iv$ is analytic, u and v are *conjugate* harmonic functions.

Example. Consider the real function $u(x, y) = \cos x \cosh y$

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\cos x \cosh y + \cos x \cosh y = 0 \quad (218)$$

hence u is harmonic. Then we find the conjugate harmonic function $v(x, y)$. Using the C-R equations

$$\frac{\partial v}{\partial y} = \frac{\partial u}{\partial x} = -\sin x \cosh y \Rightarrow v = -\sin x \sinh y + c_1(y) \quad (219)$$

$$\frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y} = -\cos x \sinh y \Rightarrow v = -\sin x \sinh y + c_2(x) \quad (220)$$

so that $c_1 = c_2 = c$ and $v(x, y) = -\sin x \sinh y + c$, where c is a constant. Hence

$$f(z) = \cos x \cosh y - i \sin x \sinh y + \tilde{c} \quad (221)$$

is analytic by construction.

5.3 Multi-Valued Functions

Example. $f(z) = z^{1/3}$. There are three related branches of $z^{1/3}$

$$\begin{cases} F_1(z) = r^{1/3}e^{i\theta/3} \\ F_2(z) = r^{1/3}e^{i\theta/3+2\pi i/3} \\ F_3(z) = r^{1/3}e^{i\theta/3+4\pi i/3} \end{cases} \quad (222)$$

with $\theta \in [-\pi, \pi]$. Each one is single valued, but discontinuous along the negative real axis. If we glue sheets together on the branch cuts, then the three sheets form a *Riemann surface*. $f(z) = z^{1/3}$ is defined on the Riemann surface on the following way

$$f(z) = F_i(z) \quad \text{on sheet } i \quad (223)$$

$f(z)$ is single valued and continuous on the Riemann surface.

Example. $f(z) = z^{1/2}$: 2 branches and 2 Riemann sheets.

Example. $f(z) = z^{1/n}$: n branches and n Riemann sheets.

Example. $f(z) = \ln z = \ln(re^{i\theta})$ not defined at $z = 0$.

$$f(z) = \ln r + i\theta + 2\pi in \quad (224)$$

has one branch for each integer n .

Example. $f(z) = (z - z_0)^{1/3}$. A *branch point* is a point that cannot be encircled without moving on to a different sheet of the Riemann surface of $f(z)$.

Example. $f(z) = (z - a)^{1/2}(z - b)^{1/2}$, $a, b \in \mathbb{R}$. The function has two branch points a and b , the branch cuts must begin or end there (see Fig.4).

5.4 Integration of Complex Functions

5.4.1 Contours

We focus on *contour integrals*, $\int_C f(z)dz$, along lines or paths C in the complex plane.

Example. Evaluate $\int_C z dz$ along (i) $y = x^2$ and (ii) $y = x$.

$$\int_C z dz = \int_C (x + iy)(dx + idy) = \int_C (x dx - y dy) + i \int_C (y dx + x dy) \quad (225)$$

$$(i) \int_0^1 \int (x dx - 2x^3 dx) + i \int_0^1 (x^2 dx + 2x^2 dx) = i$$

$$(ii) \int_0^1 (x dx - x dx) + i \int_0^1 (x dx + x dx) = i$$



Figure 4: The two possible ways to place branch cuts for $f(z) = (z - a)^{1/2}(z - b)^{1/2}$, and they form the same Riemann surface.

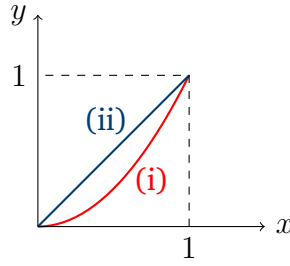


Figure 5: The two paths, (i) $y = x^2$ and (ii) $y = x$, along with the function $f(z)$ is to be integrated in the example.

5.4.2 Cauchy's Theorem

Theorem. Cauchy's theorem. If $f(z)$ is analytic everywhere on and within a closed contour C

$$\oint_C f(z) dz = 0 \quad (226)$$

Theorem. Green's theorem in the plane. P and Q are functions of x and y , and C is a closed contour in the $x - y$ plane, then

$$\oint_C (P dx + Q dy) = \iint_D \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} \right) dx dy \quad (227)$$

Proof. Proof of Cauchy's theorem

$$\begin{aligned} \oint_C f(z) dz &= \oint_C (u(x, y) + iv(x, y))(dx + idy) \\ &= \oint_C (u dx - v dy) + i \oint_C (v dx + u dy) \\ &= \iint_D \left(-\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) dx dy + i \iint_D \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y} \right) dx dy = 0 \end{aligned} \quad (228)$$

5.4.3 Path Independence

Theorem. Let C_1 and C_2 be two contours from z_a to z_b . If $f(z)$ is analytic on C_1 and C_2 and the region between them, then

$$\int_{C_1} f(z) dz = \int_{C_2} f(z) dz \quad (229)$$

Proof. Consider closed contour $C = C_1 - C_2$. By Cauchy's theorem

$$\oint_C f(z) dz = \int_{C_1} f(z) dz - \int_{C_2} f(z) dz = 0 \quad (230)$$

5.4.4 Contour Deformation

Theorem. If C_1 and C_2 are closed contours, and C_1 can be deformed into C_2 entirely in a region where $f(z)$ is analytic, then

$$\oint_{C_1} f(z)dz = \oint_{C_2} f(z)dz \quad (231)$$

Proof. Choose line segment AB as shown in the Fig.6. Consider $C = C_1 + \overline{BA} - C_2 + \overline{AB}$. By Cauchy's theorem

$$\begin{aligned} \oint_C f(z)dz &= \left(\int_{C_1} + \int_{\overline{BA}} - \int_{C_2} + \int_{\overline{AB}} \right) f(z)dz \\ &= \int_{C_1} f(z)dz - \int_{C_2} f(z)dz = 0 \end{aligned} \quad (232)$$

Example. Evaluate $\oint_{|z|=1} \frac{1}{z} dz$. Deform the contour into a small circle, radius r , centred on the origin, then

$$\oint_{|z|=1} \frac{1}{z} dz = \oint_{|z|=r} e^{-i\theta} i e^{i\theta} d\theta = 2\pi i \quad (233)$$

5.4.5 Cauchy's Integral Theorem

Theorem. If $f(z)$ is analytic within and on a closed contour C and z_0 is any point within C , then

$$\oint_C \frac{f(z)}{z - z_0} dz = 2\pi i f(z_0) \quad (234)$$

or

$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z - z_0} dz \quad (235)$$

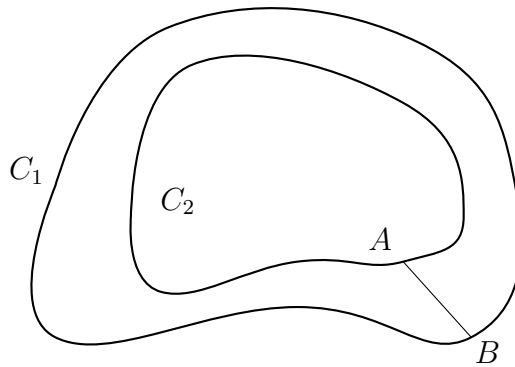
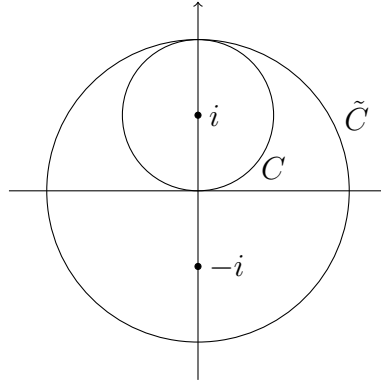


Figure 6: Caption

Figure 7: The contour C and \tilde{C} .

Proof. The integral is analytic within and on C except at $z = z_0$. Let C_r be a small circle around z_0 , i.e. $C_r : z = z_0 + re^{i\theta}$, then

$$\begin{aligned} \oint_C \frac{f(z)}{z - z_0} dz &= \oint_{C_r} \frac{f(z)}{z - z_0} dz = \int_0^{2\pi} \frac{f(z_0 + re^{i\theta})}{re^{i\theta}} ire^{i\theta} d\theta \\ &= i \int_0^{2\pi} f(z_0 + re^{i\theta}) d\theta = \lim_{r \rightarrow 0} i \int_0^{2\pi} f(z_0 + re^{i\theta}) d\theta = 2\pi i f(z_0) \end{aligned} \quad (236)$$

Example. Consider the integral

$$\oint \frac{\sin z}{z^2 + 1} dz = \oint_C \frac{\sin z}{(z + i)(z - i)} dz \quad (237)$$

and consider the closed contour C and \tilde{C} , which are showed in Fig.7. For the contour C , We choose

$$f(z) = \frac{\sin z}{z + i} \quad (238)$$

Then

$$\oint_C \frac{\sin z}{z^2 + 1} dz = \oint_C \frac{f(z)}{z - i} dz = 2\pi i \frac{\sin i}{2i} = \pi i \sinh 1 \quad (239)$$

\tilde{C} is a circle of radius 2 centred at origin, so

$$\begin{aligned} \oint_{\tilde{C}} \frac{\sin z}{z^2 + 1} dz &= \oint_{\tilde{C}} \frac{\sin z}{(z + i)(z - i)} dz = \frac{i}{2} \oint_{\tilde{C}} \left(\frac{\sin z}{z + i} - \frac{\sin z}{z - i} \right) dz \\ &= -\pi (\sin(-i) - \sin(i)) = 2\pi i \sinh 1 \end{aligned} \quad (240)$$

5.4.6 Derivatives of Analytic Functions

Cauchy's integral theorem gives

$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z - z_0} dz \quad (241)$$

If we differentiate both sides of Cauchy's integral formula with respect to z_0 , interchanging the orders of integration and differentiation, we get

$$f'(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^2} dz \quad (242)$$

Similarly,

$$f''(z_0) = \frac{2!}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^3} dz \quad (243)$$

\vdots

$$f^{(n)}(z_0) = \frac{n!}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^{n+1}} dz \quad (244)$$

Example.

$$\oint_C \frac{1}{z^n} dz \quad \text{with} \quad C : |z| = r \quad (245)$$

- $n = 1, \oint_C (1/z) dz = 2\pi i$
- $n \geq 2, \oint_C (1/z) dz = 0$

5.4.7 Fourier Transform of a Gaussian

We have known that

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \int_{-\infty}^{\infty} e^{-(x'+ia)^2} dx' \quad (246)$$

where a is a real number. Now we use Cauchy's theorem to prove it.

Proof.

$$I_1 = \int_{-\infty}^{\infty} e^{-x^2} dx = \int_{C_1} e^{-z^2} dz \quad (247)$$

$$I_2 = \int_{-\infty}^{\infty} e^{-(x'+ia)^2} dx' = \int_{C_2} e^{-z^2} dz \quad (248)$$

where C_1 is the whole x -axis and C_2 is the line parallel to the x -axis at $z = x + ia$. Let's assume $a > 0$. To begin with, we construct a closed contour $C_R = C_{2R} + E_R^+ - C_{1R} + E_R^-$ (see in Fig.8).

$$\oint_{C_R} e^{-z^2} dz = 0 \quad (249)$$

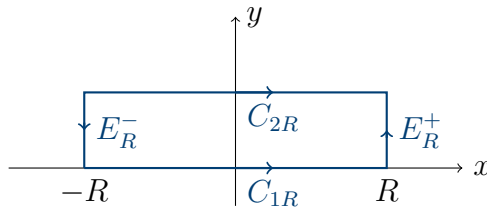


Figure 8: The contour C_R .

for any R . When $R \rightarrow \infty$, then

$$\lim_{R \rightarrow \infty} \oint_{C_R} e^{-z^2} dz = \lim_{R \rightarrow \infty} \left(\int_{C_1} + \int_{E_R^+} - \int_{C_2} + \int_{E_R^-} \right) e^{-z^2} dz = I_1 - I_2 = 0 \quad (250)$$

5.5 Power Series Representations of Complex Functions

5.5.1 Taylor Series

$f(z)$ is analytic at z_0 if it has a Taylor series in a neighbourhood of z_0

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n \quad (251)$$

where

$$a_n = \frac{f^{(n)}(z_0)}{n!} = \frac{1}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^{n+1}} dz \quad (252)$$

5.5.2 Singularities

If $f(z)$ is analytic except at specific points in the complex plane, those points are called isolated singularities or *poles*.

Example.

$$f(z) = \frac{e^z}{(z - 5)(z + i)(z - (1 + i))^2} \quad (253)$$

has isolated singularities at $z = 5, i, 1 + i$.

There two types of singularities:

1. $f(z)$ has a *pole of order* $m (m \geq 1)$ at z_0 if there exists a $g(z)$ which is analytic at z_0 and $g(z_0) \neq 0$ s.t.

$$f(z) = \frac{g(z)}{(z - z_0)^m} \quad (254)$$

This implies $f(z)$ has a power series except around z_0

$$f(z) = \sum_{n=-m}^{\infty} a_n (z - z_0)^n \quad (255)$$

Poles of order 1 are called *single poles*.

2. $f(z)$ has an *essential singularity* at z_0 if $f(z)$ has a power series except around $z = z_0$ with infinitely many negative powers

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n \quad (256)$$

Example.

$$f(z) = e^{1/z} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{z} \right)^n \quad (257)$$

5.6 Contour Integration using the Residue Theorem

5.6.1 The Residue Theorem

Definition. Let f has an isolated singularity at z_0 , then the residue of f at z_0 is

$$\text{Res}_f(z_0) = \frac{1}{2\pi i} \oint_{C_{z_0}} f(z) dz \quad (258)$$

where C_{z_0} is a closed contour s.t. z_0 is inside and $f(z)$ is analytic inside except at z_0 . If $f(z)$ has a pole of order m at z_0 , then

$$f(z) = \frac{g(z)}{(z - z_0)^m} \quad (259)$$

and

$$\text{Res}_f(z_0) = \frac{1}{2\pi i} \oint_C \frac{g(z)}{(z - z_0)^m} dz = \frac{1}{(m-1)!} \left. \frac{d^{m-1}g(z)}{dz^{m-1}} \right|_{z=z_0} \quad (260)$$

Example.

$$(1) f(z) = 1/(z - z_0)$$

$$\text{Res}_f(z_0) = 1 \quad (261)$$

$$(2) f(z) = \sin z / (1 + z)^2$$

$$\text{Res}_f(-1) = \left. \frac{d \sin z}{dz} \right|_{z=-1} = \cos(-1) = \cos 1 \quad (262)$$

Theorem. Let C is a closed contour, $f(z)$ is a function that is analytic on C and inside C except at $z = z_1, \dots, z_N$. Then

$$\oint_C f(z) dz = 2\pi i \sum_{k=1}^N \text{Res}_f(z_k) \quad (263)$$

Proof. By Cauchy's theorem

$$\oint_{\hat{C}} f(z) dz = \oint_C f(z) dz - 2\pi i \sum_{k=1}^N \text{Res}_f(z_k) = 0 \quad (264)$$

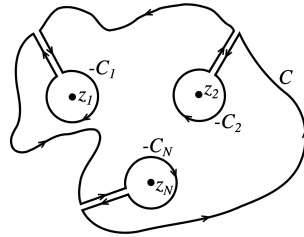


Figure 9: The contour C used in the proof of the residue theorem.

5.6.2 Contour Integration Examples

Example. 1

$$\begin{aligned}
I &= \oint_{|z|=1} e^{1/z} dz \\
&= \oint_{|z|=1} \left[1 + \frac{1}{z} + \frac{1}{2!} \left(\frac{1}{z} \right)^2 + \cdots \right] dz = 2\pi i
\end{aligned} \tag{265}$$

Example. 2

$$\begin{aligned}
I &= \oint_{|z|=3} \frac{z+2}{2z^2+1} dz = \oint_{|z|=3} \frac{z+2}{2(z^2+1/2)} dz \\
&= \oint_{|z|=3} \frac{z+2}{2(z+\frac{i}{\sqrt{2}})(z-\frac{i}{\sqrt{2}})} dz \\
&= 2\pi i \left[\text{Res} \left(\frac{i}{\sqrt{2}} \right) + \text{Res} \left(-\frac{i}{\sqrt{2}} \right) \right] \\
&= 2\pi i \left[\frac{\frac{i}{\sqrt{2}}+2}{2(\frac{i}{\sqrt{2}}+\frac{i}{\sqrt{2}})} + \frac{-\frac{i}{\sqrt{2}}+2}{2(-\frac{i}{\sqrt{2}}-\frac{i}{\sqrt{2}})} \right] = \pi i
\end{aligned} \tag{266}$$

Example. 3

$$I = \int_{-\infty}^{\infty} \frac{dx}{(x^2+1)(x^2+9)} \tag{267}$$

Consider the contour $C = C_R + S_R$ (see in fig.10(a)), we have

$$\begin{aligned}
I &= \lim_{R \rightarrow \infty} \int_{-R}^R \frac{dx}{(x^2+1)(x^2+9)} \\
&= \lim_{R \rightarrow \infty} \oint_C \frac{dz}{(z+i)(z-i)(z+3i)(z-3i)} - \lim_{R \rightarrow \infty} \int_{C_R} \frac{dz}{(z^2+1)(z^2+9)} \\
&= 2\pi i [\text{Res}(i) + \text{Res}(3i)] - 0 \\
&= 2\pi i \left(\frac{1}{16i} + \frac{1}{-48i} \right) = \frac{\pi}{12}
\end{aligned} \tag{268}$$

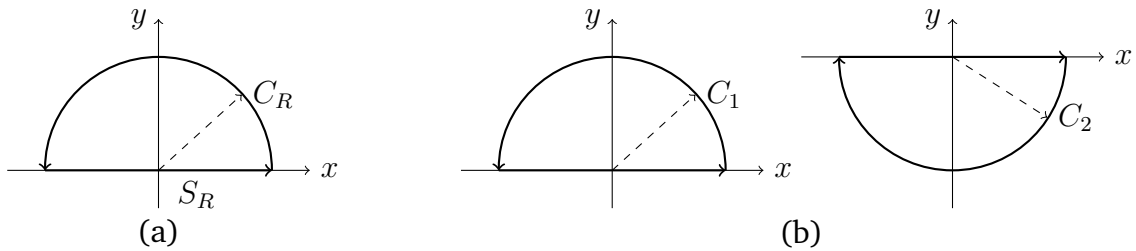


Figure 10: (a) The contour for example 3. (b) The contour for example 4.

Example. 4

$$\begin{aligned}
I &= \int_{-\infty}^{\infty} \frac{\cos x}{x^2 + 1} dx = \int_{x\text{-axis}} \frac{\cos z}{z^2 + 1} dz \\
&= \int_{x\text{-axis}} \frac{e^{iz}}{2(z+i)(z-i)} dz + \int_{x\text{-axis}} \frac{e^{-iz}}{2(z+i)(z-i)} dz \\
&= I_1 + I_2
\end{aligned} \tag{269}$$

Consider the contour C_1 and C_2 (see in fig.10(b))

$$\begin{aligned}
I_1 &= \lim_{R \rightarrow \infty} \oint_C \frac{e^{iz}}{2(z+i)(z-i)} dz - \lim_{R \rightarrow \infty} \int_{C_1} \frac{e^{iz}}{2(z+i)(z-i)} dz \\
&= 2\pi i \operatorname{Res}(i) - \lim_{R \rightarrow \infty} \int_{C_1} \frac{e^{ix-y}}{2(z+i)(z-i)} dz \\
&= 2\pi i \frac{e^{-1}}{4i} - 0 = \frac{\pi}{2} e^{-1}
\end{aligned} \tag{270}$$

$$\begin{aligned}
I_2 &= - \lim_{R \rightarrow \infty} \oint_C \frac{e^{-iz}}{2(z+i)(z-i)} dz - \lim_{R \rightarrow \infty} \int_{C_2} \frac{e^{-iz}}{2(z+i)(z-i)} dz \\
&= -2\pi i \operatorname{Res}(-i) - \lim_{R \rightarrow \infty} \int_{C_2} \frac{e^{-ix+y}}{2(z+i)(z-i)} dz \\
&= -2\pi i \frac{e^{-1}}{-4i} - 0 = \frac{\pi}{2} e^{-1}
\end{aligned} \tag{271}$$

So we have

$$I = I_1 + I_2 = \pi e^{-1} \tag{272}$$

5.6.3 Inverting Laplace Transforms

Suppose

$$F(s) = \text{LT}[f(t)] = \int_0^s f(t)e^{-st} dt \tag{273}$$

where $t > 0$, then

$$f(t) = \text{LT}^{-1}[F(s)] = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} F(s)e^{st} ds \tag{274}$$

which is called *Bromwich integral*. To invert a Laplace transform $F(s)$

- (i) Find the singular points a_1, a_2, \dots , of $F(s)$ and choose a real number c such that $c > \operatorname{Re}(a_i)$ for all i .
- (ii) Close the Bromwich integral contour show in fig.11 with a large semicircle in the left-hand half-plane.
- (iii) If the integral around the semicircle vanished as $R \rightarrow \infty$, then

$$f(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} F(s)e^{st} ds = \sum_i \operatorname{Res}(a_i), \quad (t > 0) \tag{275}$$

where $\operatorname{Res}(a_i)$ is the residues of $F(s)e^{st}$.

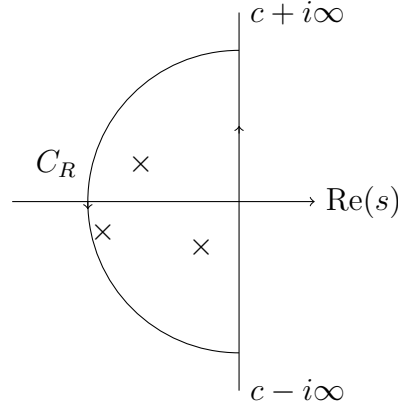


Figure 11: The contour for inverting Laplace transforms.

6 Calculus of Variations

- A **function** f maps a number, x , to another number, $f(x)$.
- A **functional** I maps a function, f , to a number $I[f]$.

Example.

$$(a) \quad I[f] = \frac{1}{b-a} \int_a^b f(x) dx$$

$$(b) \quad T(\psi) = \int \psi^*(x) \frac{\hat{p}^2}{2m} \psi(x) dx$$

$$(c) \quad U(\rho) = \frac{1}{2} \iint \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{4\pi\epsilon_0|\mathbf{r}-\mathbf{r}'|} d^3\mathbf{r} d^3\mathbf{r}'$$

$$(d) \quad S[y] = \int_a^b \sqrt{1 + \left(\frac{dy}{dx}\right)^2} dx = \text{length of curve from } x = a \text{ to } x = b \text{ given by } y(x).$$

$$(e) \quad S[x] = \int_{t_1}^{t_2} \left[\frac{1}{2} m \dot{x}^2 - V(x) \right] dt = \text{action}.$$

6.1 The Euler-Lagrange Problem

Let y be a function of variable $y(x)$

$$I[y] = \int_{x_A}^{x_B} f(x, y(x), y'(x)) dx \quad (276)$$

where f is a function of 3 arguments, and $x_A, x_B, y(x_A), y(x_B)$ are fixed. *Euler-Lagrange problem* is to find $y(x)$ such that $\delta I = \mathcal{O}(\delta y^2)$ at $y(x)$, and we say y extremises $I[y]$ or $I[y]$ is stationary at y .

Consider varying $y(x)$ slightly

$$y(x) \rightarrow y(x) + \delta y(x) \quad (277)$$

then

$$\begin{aligned} I[y + \delta y] &= \int_{x_A}^{x_B} f(x, y(x) + \delta y(x), y' + \delta y'(x)) dx \\ &= \int_{x_A}^{x_B} \left[f(x, y, y') + \delta y \frac{\partial f}{\partial y} + \delta y' \frac{\partial f}{\partial y'} + \mathcal{O}(\delta y^2) \right] dx \end{aligned} \quad (278)$$

so we have

$$\begin{aligned} \delta I &= I[y + \delta y] - I[y] \\ &= \int_{x_A}^{x_B} \left(\delta y \frac{\partial f}{\partial y} + \delta y' \frac{\partial f}{\partial y'} \right) dx + \mathcal{O}(\delta y^2) \\ &= \int_{x_A}^{x_B} \left(\delta y \frac{\partial f}{\partial y} \right) dx + \left[\delta y \frac{\partial f}{\partial y'} \right]_{x_A}^{x_B} - \int_{x_A}^{x_B} \delta y \frac{d}{dx} \left(\frac{\partial f}{\partial y'} \right) dx + \mathcal{O}(\delta y^2) \\ &= \int_{x_A}^{x_B} \delta y \left[\frac{\partial f}{\partial y} - \frac{d}{dx} \left(\frac{\partial f}{\partial y'} \right) \right] dx + \mathcal{O}(\delta y^2) \end{aligned} \quad (279)$$

$\delta I = \mathcal{O}(\delta y^2)$ if and only if

$$\boxed{\frac{\partial f}{\partial y} - \frac{d}{dx} \left(\frac{\partial f}{\partial y'} \right) = 0} \quad (280)$$

for $x_A \leq x \leq x_B$. This equation is called *Euler-Lagrange equation*.

Example.

$$f(x, y, y') = (1 + x^2)y'^2 - y^4 \quad (281)$$

$I[y] = \int_{x_A}^{x_B} f(x, y, y') dx$ is stationary if

$$-4y^3 - \frac{d}{dx} [(1 + x^2)2y'] = 0 \quad (282)$$

6.1.1 Beltrami identity

Suppose $f(x, y, y') = f(y, y')$, then

$$\frac{df}{dx} = \frac{\partial f}{\partial y} \frac{dy}{dx} + \frac{\partial f}{\partial y'} \frac{dy'}{dx} \quad (283)$$

if y is a solution of the Euler-Lagrange equation

$$\frac{df}{dx} = \frac{d}{dt} \left(\frac{\partial f}{\partial y'} \right) y' + \frac{\partial f}{\partial y'} \frac{dy'}{dx} = \frac{d}{dx} \left(\frac{\partial f}{\partial y'} y' \right) \quad (284)$$

Then

$$\frac{d}{dx} \left(f - \frac{\partial f}{\partial y'} y' \right) = 0 \quad \Rightarrow \quad \boxed{f - \frac{\partial f}{\partial y'} y' = \text{const}} \quad (285)$$

with the condition $\partial f / \partial x = 0$. This equation is called *Beltrami identity*, which is the first integral of Euler-Lagrange equation.

Example.

$$I[y] = \int f dx \quad \text{with} \quad f(y, y') = y'^2 - y^4 \quad (286)$$

Applying the Beltrami identity

$$y'^2 - y^4 - 2y'^2 = \text{const} \quad (287)$$

6.1.2 Functional Derivatives

We know that

$$\delta I = \int_{x_A}^{x_B} \delta y \left[\frac{\partial f}{\partial y} - \frac{d}{dx} \left(\frac{\partial f}{\partial y'} \right) \right] dx + \mathcal{O}(\delta y^2) \quad (288)$$

then we can define the *functional derivative* of I

$$\frac{\delta I}{\delta y(x)} = \frac{\partial f}{\partial y} - \frac{d}{dx} \left(\frac{\partial f}{\partial y'} \right) \quad (289)$$

then Euler-Lagrange equation can be written as

$$\frac{\delta I}{\delta y(x)} = 0 \quad (290)$$

6.1.3 Lagrangian Mechanics

The Lagrangian of a classical particle moving in three dimensions is

$$L = T - V = \frac{1}{2} m \dot{\mathbf{x}}^2 + V(\mathbf{x}, t) \quad (291)$$

where $\mathbf{x} = (x_1, x_2, x_3)$. The action

$$S[\mathbf{x}(t)] = \int_{t_A}^{t_B} L(t, \mathbf{x}, \dot{\mathbf{x}}) \quad (292)$$

Vary $S[\mathbf{x}]$ separately for x_1, x_2, x_3 and get an Euler-Lagrange equation for each

$$\frac{\partial L}{\partial x_i} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}_i} \right) = 0, \quad i = 1, 2, 3 \quad (293)$$

i.e.

$$m \ddot{x}_i = -\nabla_i V \quad (294)$$

which is Newton's equation.

6.1.4 Euler-Lagrange Examples

(a) Shortest Path Problem

Method 1

Between (x, y) and $(x + dx, y + dy)$ along curve $y(x)$, the distance is

$$ds = \sqrt{dx^2 + dy^2} = \sqrt{1 + \left(\frac{dy}{dx}\right)^2} dx \quad (295)$$

so the length of $y(x)$ is

$$\int ds = \int_{x_A}^{x_B} \sqrt{1 + y'^2} dx \quad (296)$$

This extremised by Euler-Lagrange equation

$$0 - \frac{d}{dx} \left(\frac{y'}{\sqrt{1 + y'^2}} \right) = 0 \Rightarrow y' = c \Rightarrow y = cx + d \quad (297)$$

Method 2

We write the curve in *parametrised* form

$$y = y(\lambda), \quad x = x(\lambda) \quad (298)$$

The curve fixed at $\lambda = \lambda_A$ at (x_A, y_A) and $\lambda = \lambda_B$ at (x_B, y_B) . The length of path is

$$\int ds = \int_{\lambda_A}^{\lambda_B} \sqrt{\left(\frac{dx}{d\lambda}\right)^2 + \left(\frac{dy}{d\lambda}\right)^2} d\lambda \quad (299)$$

This extremised by Euler-Lagrange equation. For x

$$0 - \frac{d}{d\lambda} \left(\frac{x'}{\sqrt{x'^2 + y'^2}} \right) = 0 \Rightarrow \frac{x'}{\sqrt{x'^2 + y'^2}} = \alpha \quad (300)$$

Similarly, for y

$$0 - \frac{d}{d\lambda} \left(\frac{y'}{\sqrt{x'^2 + y'^2}} \right) = 0 \Rightarrow \frac{y'}{\sqrt{x'^2 + y'^2}} = \beta \quad (301)$$

So we have

$$\frac{y'}{x'} = \gamma \Rightarrow \frac{dy}{dx} = \gamma \Rightarrow y = \gamma x + c \quad (302)$$

(b) Brachistochrone

A particle moving from $A(0, 0)$ to $B(x_B, y_B)$ takes the time

$$T = \int_A^B dt = \int_A^B \frac{ds}{v} = \int_{x=0}^{x=x_B} \frac{\sqrt{1 + y'^2}}{\sqrt{2gy}} dx \quad (303)$$

Using the Beltrami identity

$$\frac{\sqrt{1+y'^2}}{\sqrt{2gy}} - \frac{y'}{\sqrt{1+y'^2}} y' = c \Rightarrow y(1+y'^2) = c^2 \Rightarrow y' = \frac{\alpha - y}{y} \quad (304)$$

where $\alpha = c^2$. The solution is a cycloid

$$x = x(\theta) = a(\theta - \sin \theta) \quad (305)$$

$$y = y(\theta) = a(1 - \cos \theta) \quad (306)$$

where $a = \alpha/2$. Then the total time

$$T = \int_0^{\theta_B} \frac{\sqrt{(dx/d\theta)^2 + (dy/d\theta)^2}}{\sqrt{2gy}} d\theta = \int_0^{\theta_B} \sqrt{\frac{a}{g}} d\theta = \sqrt{\frac{a}{g}} \theta_B \quad (307)$$

6.1.5 Symmetries and Conservation

- **Conservation of Energy**

Consider a single particle in 1D space, and the potential doesn't depend explicitly on time t . The Lagrangian

$$L(x, \dot{x}) = T - V = \frac{1}{2} m \dot{x}^2 - V(x) \quad (308)$$

We use the Beltrami identity

$$\begin{aligned} L - \frac{\partial L}{\partial \dot{x}} \dot{x} &= \text{const} \\ -\left(\frac{1}{2} m \dot{x}^2 + V\right) &= \text{const} \\ T + V &= \text{const} \end{aligned} \quad (309)$$

so we see that the V being independent of t leads to the conservation of total energy. More generally, for any mechanical system with position variables $\mathbf{q} = (q_1, q_2, \dots, q_N)$

$$L(\mathbf{q}, \dot{\mathbf{q}}) = T - V(\mathbf{q}) \quad (310)$$

which does not depend on t . If one defines

$$H = -L + \sum_{i=1}^N \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} \quad (311)$$

H is the classical Hamiltonian and the total energy. Then the Beltrami identity tells us that this is a constant of the motion.

- **Conservation of Momentum**

Consider a particle in 3D space. Suppose the potential $V(\mathbf{x}, \dot{\mathbf{x}}, t)$ is independent of $\mathbf{x} = (x_1, x_2, x_3)$, i. e.

$$\frac{\partial V}{\partial x_i} = 0, \quad i = 1, 2, 3 \quad (312)$$

The Lagrangian

$$L = T - V = \frac{1}{2}m \left(\sum_i \dot{x}_i^2 \right) - V \quad (313)$$

The Euler-Lagrange equation gives

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{x}_i} \right) = 0 \quad \Rightarrow \quad m\dot{x}_i = \text{const} \quad (314)$$

which is the momentum of that particle in the i direction.

- **Conservation of Angular Momentum**

Suppose $\mathbf{q} = (r(t), \theta(t), \phi(t))$, then the Lagrangian for the particle is

$$L = T - V(r, \theta, \phi) \quad (315)$$

where the kinetic energy

$$T = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2 + r^2 \sin^2 \theta \dot{\phi}^2) \quad (316)$$

We find that T doesn't depend on ϕ . If V also doesn't depend on ϕ , then the Lagrangian doesn't depend on ϕ .

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\phi}} \right) = \frac{\partial L}{\partial \phi} = 0 \quad \Rightarrow \quad mr^2 \sin^2 \theta \dot{\phi} = \text{const} \quad (317)$$

is a constant of the motion. This is the angular momentum in the z -direction. If the potential V is a function of r alone, the system is spherically symmetric, then all components of the angular momentum are conserved.

6.2 Constrain Optimisation and Lagrange Multipliers

6.2.1 Constrained Optimisation of Functions

Consider the function $f(x, y)$ and we want to find the stationary points of f subject to the constraint

$$g(x, y) - C = 0 \quad (318)$$

At the stationary point P , the contour of $f(x, y)$ are parallel to the curve $g(x, y) = C$

$$\nabla f|_P \parallel \nabla g|_P \quad \Rightarrow \quad \nabla (f(x, y) - \lambda g(x, y))|_P = 0 \quad (319)$$

The gradient ratio λ , is called a *Lagrange multiplier*. This equation has two components.

In d -dimension with the function $f(x_1, \dots, x_d)$ and constraint $g(x_1, \dots, x_d) = C$. With more constraints

$$\begin{aligned} g_1(\mathbf{x}) &= C_1 \\ g_2(\mathbf{x}) &= C_2 \\ &\vdots \\ g_k(\mathbf{x}) &= C_k \end{aligned} \quad (320)$$

constraint surface is $n - k$ dimension. f is constrained on the constraint surface if

$$\nabla(f - \lambda_1 g_1 - \lambda_2 g_2 - \cdots - \lambda_k g_k) = 0 \quad (321)$$

Example. Find the minimum distance between curves $xy = 1$ and $x + 2y = 1$. Our task is to minimise $\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$, which is the same problem as minimising

$$f(x_1, x_2, y_1, y_2) = (x_2 - x_1)^2 + (y_2 - y_1)^2 \quad (322)$$

Solve $\nabla u = 0$, where

$$u(x_1, x_2, y_1, y_2) = f(x_1, x_2, y_1, y_2) + \lambda_1 x_1 y_1 + \mu(x_2 + 2y_2) \quad (323)$$

Unconstrained minimisation of $u(x_1, x_2, y_1, y_2)$ gives

$$\frac{\partial u}{\partial x_1} = 2(x_1 - x_2) + \lambda_1 y_1 = 0 \quad (324)$$

$$\frac{\partial u}{\partial x_2} = 2(x_2 - x_1) + \mu_2 = 0 \quad (325)$$

$$\frac{\partial u}{\partial y_1} = 2(y_1 - y_2) + \lambda_1 x_1 = 0 \quad (326)$$

$$\frac{\partial u}{\partial y_2} = 2(y_2 - y_1) + 2\mu_2 = 0 \quad (327)$$

The solution is

$$(x_1, y_1) = \left(\sqrt{2}, \frac{\sqrt{2}}{2} \right), \quad (x_2, y_2) = \left(\frac{1 + 3\sqrt{2}}{5}, \frac{4 - 3\sqrt{2}}{10} \right) \quad (328)$$

The minimum distance is then $(2\sqrt{2} - 1)/\sqrt{5}$

6.2.2 Constrained Optimisation of Functionals

Functional problem is to extremise $F[y]$ subject to $G[y] = C$. The Lagrange multiplier is to find solutions of $\delta(F - \lambda G) = 0$.

Example. The catenary: Find the shape formed by a heavy rope of a chain hanging between two fixed end points $A(-a, 0)$ and $B(a, 0)$. Our task is to minimise the total energy. Suppose the mass density is ρ , and the mass of piece is $dm = \rho ds$. The total energy

$$E = g \int_A^B y dm = \rho g \int_A^B y ds = \rho g \int_{-a}^a y \sqrt{1 + \left(\frac{dy}{dx} \right)^2} dx \quad (329)$$

The length of the rope is fixed. So the constraint

$$L = \int_A^B ds = \int_{-a}^a \sqrt{1 + \left(\frac{dy}{dx} \right)^2} dx \quad (330)$$

Then we have to extremise

$$\begin{aligned}
 U = E - \lambda L &= \rho g \int_{-a}^a y \sqrt{1 + \left(\frac{dy}{dx}\right)^2} dx - \lambda \int_{-a}^a \sqrt{1 + \left(\frac{dy}{dx}\right)^2} dx \\
 &= \int_{-a}^a (\rho g y - \lambda) \sqrt{1 + y'^2} dx = \int_{-a}^a f dx
 \end{aligned} \tag{331}$$

f does not depend on x , then we can use Beltrami identity

$$f - \frac{\partial f}{\partial y'} y' = C \tag{332}$$

which is

$$(\rho g y - \lambda) \sqrt{1 + y'^2} - (\rho g y - \lambda) \frac{y'^2}{\sqrt{1 + y'^2}} = C \tag{333}$$

$$\rho g y - \lambda = C \sqrt{1 + y'^2} \tag{334}$$

Let $\eta = \rho g y - \lambda$, then we have $\eta' = \rho g y'$. Hence

$$\eta = C \sqrt{1 + \frac{\eta'^2}{\rho^2 g^2}}, \quad \eta' = \pm \rho g \sqrt{\frac{\eta^2}{C^2} - 1} \tag{335}$$

For $x \geq 0$, $\eta' \geq 0$. So

$$\eta' = \frac{d\eta}{dx} = \rho g \sqrt{\frac{\eta^2}{C^2} - 1} \Rightarrow \frac{d\eta}{\sqrt{\frac{\eta^2}{C^2} - 1}} = \rho g dx \tag{336}$$

Let $\eta = C \cosh q$, then $d\eta = C \sinh q dq$

$$\begin{aligned}
 \int \frac{d\eta}{\sqrt{\frac{\eta^2}{C^2} - 1}} &= \rho g \int dx \\
 \Rightarrow C \int dq &= \rho g dx \\
 \Rightarrow Cq &= \rho g x + d \\
 \Rightarrow \frac{\eta}{C} &= \cosh \left(\frac{\rho g x + d}{C} \right)
 \end{aligned} \tag{337}$$

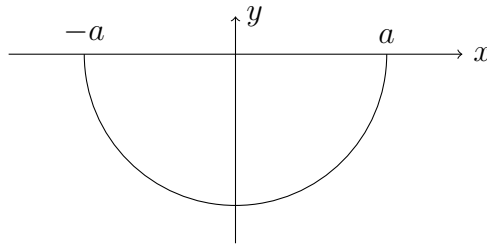


Figure 12: A heavy rope of a chain hanging between two fixed end points $A(-a, 0)$ and $B(a, 0)$.

$\eta' = 0$ when $x = 0$, so $d = 0$. Then

$$y(x) = \frac{1}{\rho g} \left[\cosh \left(\frac{\rho g x}{C} \right) + \lambda \right] \quad (338)$$

The two constraints

1. When $x = \pm a$, $y = 0$

$$\frac{1}{\rho g} \left[\cosh \left(\frac{\rho g a}{C} + \lambda \right) \right] = 0 \quad (339)$$

2. The length of the rope is fixed

$$\begin{aligned} L &= \int_{-a}^a \sqrt{1 + y'^2} dx = \int_{-a}^a \cosh \left(\frac{\rho g x}{C} \right) dx \\ &= \frac{C}{\rho g} \sinh \frac{\rho g x}{C} \Big|_{-a}^a = \frac{2C}{\rho g} \sinh \frac{\rho g a}{C} \end{aligned} \quad (340)$$

Find numerically solutions for C and λ from the constraints above.

6.3 Variation Methods for Solving the Schrödinger Equation

The problem of finding the eigenfunctions of a Hamiltonian \hat{H} is equivalent to the problem of finding the stationary points of the functional

$$E[\psi] = \int \psi^* \hat{H} \psi \quad (341)$$

subject to the normalisation constraint

$$\int \psi^* \psi = 1 \quad (342)$$

We claim that

$$I[\psi] = \int \psi^* \hat{H} \psi - \varepsilon \int \psi^* \psi \quad (343)$$

Here ε is the eigenvalue. Let ψ extremes I

$$\begin{aligned} \delta I &= I[\psi + \delta\psi] - I[\psi] \\ &= \int (\delta\psi^*) \hat{H} \psi + \int \psi^* \hat{H} (\delta\psi) - \varepsilon \int (\delta\psi^*) \psi - \varepsilon \int \psi^* (\delta\psi) \\ &= \int (\delta\psi^*) (\hat{H} \psi - \varepsilon \psi) + \int (\delta\psi) (\hat{H} \psi - \varepsilon \psi)^* = 0 \end{aligned} \quad (344)$$

$$\begin{aligned} \delta I &= I[\psi + i\delta\psi] - I[\psi] \\ &= -i \int (\delta\psi^*) \hat{H} \psi + i \int \psi^* \hat{H} (\delta\psi) + i\varepsilon \int (\delta\psi^*) \psi - i\varepsilon \int \psi^* (\delta\psi) \\ &= -i \int (\delta\psi^*) (\hat{H} \psi - \varepsilon \psi) + i \int (\delta\psi) (\hat{H} \psi - \varepsilon \psi)^* = 0 \end{aligned} \quad (345)$$

So we have

$$\int (\delta\psi^*)(\hat{H}\psi - \varepsilon\psi) = 0 \quad (346)$$

for any ψ . Hence

$$\hat{H}\psi - \varepsilon\psi = 0 \quad (347)$$

6.3.1 The Linear Variational Method

Choose a finite set of basis functions $\{\phi_1, \dots, \phi_M\}$. The basis are linear independent, but may not be orthogonal. Express ψ as a linear combination

$$\tilde{\psi}(\mathbf{c}) = \sum_{\alpha=1}^M c_{\alpha} \phi_{\alpha} \quad (348)$$

where $\mathbf{c} = (c_1, \dots, c_M)$ is an M -dimensional vector of expansion coefficients to be determine.

$$I[\tilde{\psi}] = I[\mathbf{c}] = E[\mathbf{c}] - \varepsilon N[\mathbf{c}] \quad (349)$$

where

$$E[\mathbf{c}] = \int \sum_{\alpha=1}^M c_{\alpha}^* \phi_{\alpha}^* \hat{H} \sum_{\beta=1}^M c_{\beta} \phi_{\beta} = \sum_{\alpha,\beta=1}^M c_{\alpha}^* H_{\alpha\beta} c_{\beta} \quad (350)$$

where

$$H_{\alpha\beta} = \int \phi_{\alpha}^* \hat{H} \phi_{\beta} \quad (351)$$

and

$$N[\mathbf{c}] = \int \sum_{\alpha} c_{\alpha}^* \phi_{\alpha}^* \sum_{\beta} c_{\beta} \phi_{\beta} = \int \sum_{\alpha,\beta=1}^M c_{\alpha}^* S_{\alpha\beta} c_{\beta} \quad (352)$$

where $S_{\alpha\beta} = \int \phi_{\alpha}^* \phi_{\beta} = \delta_{\alpha\beta}$ if basis are orthogonal. Otherwise $S_{\alpha\beta}$ is a positive definite Hermitian matrix. Now we have constrained variational problem for a function of M variables.