Imperial College London

NOTES

IMPERIAL COLLEGE LONDON

DEPARTMENT OF PHYSICS

Mathematical Methods for Physicists

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Happy New Year :D

Contents

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**: $\forall \boldsymbol{u}, \boldsymbol{v} \in \mathbb{V} \Rightarrow \boldsymbol{u} + \boldsymbol{v} \in \mathbb{V}$.*
2. *$\mathbb{V}$ is closed under **scalar multiplication**: $\forall \boldsymbol{u} \in \mathbb{V}$ and $\forall$ scalar $\lambda \Rightarrow \lambda \boldsymbol{u} \in \mathbb{V}$.*

Example.

(1) 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) 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 $\boldsymbol{v}$ in $\mathbb{V}$ can be represented as a linear combination of the basis vectors

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

1.1.4 Inner Product and Orthogonality

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

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

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

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

Example.

(1) For $\mathbb{R}^3$, the inner product of (a, b, c) and (d, e, f)

$$\left\langle \begin{pmatrix} a \\ b \\ c \end{pmatrix}, \begin{pmatrix} d \\ e \\ f \end{pmatrix} \right\rangle = ad + be + cf \tag{2}$$

(2) For $\mathbb{C}^2$, the inner product of (a, b) and (c, d)

$$\left\langle \begin{pmatrix} a \\ b \end{pmatrix}, \begin{pmatrix} c \\ d \end{pmatrix} \right\rangle = a^*c + b^*d \tag{3}$$

Definition. *The **norm** of a vector is defines as* $\|\boldsymbol{v}\| = \sqrt{\langle \boldsymbol{v}, \boldsymbol{v} \rangle}$.

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

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle = 0 \tag{4}$$

A set of vectors $\{e_1, \cdots, e_n\}$ is **orthonormal** if

$$\langle e_i, e_j \rangle = \delta_{ij} = \begin{cases} 0, & i \neq j \\ 1, & i = j \end{cases} \tag{5}$$

where δ_{ij} is named as Kronecker delta.

1.2 Matrices

1.2.1 Summation Convention

Example.

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

(2) $u_i = \sum_j A_{ij}v_j = A_{ij}v_j$

This shorthand is known as the *Einstein summation convention*. In the example (1), 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*.

Example. Let $g : \mathbb{V} \to \mathbb{W}$ be a linear map. Let $\{e_1, \cdots, e_n\}$ be a basis for $\mathbb{V}$ and $\{f_1, \cdots, f_n\}$ be a basis for $\mathbb{W}$, then

$$g(e_i) = \sum_{j=1}^{n} g_{ij}f_j = g_{ij}f_j \tag{6}$$

Let $\underline{v} \in \mathbb{V}$, $\underline{v} = v_ie_i$, then

$$g(\underline{v}) = g(v_ie_i) = \sum_{i=1}^{n} v_ig(e_i) = v_ig_{ij}f_j = \omega_jf_j = \underline{\omega} \in \mathbb{W} \tag{7}$$

1.2.2 Recall Special Square Matrices

- **Unit matrix** $\mathbb{1}$. $\mathbb{1}_{ij} = \delta_{ij}$.
- **Unitary matrix.** U is unitary if $UU^\dagger = U^\dagger U = \mathbb{1}$
- **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.**
  - 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

$$R^TR = RR^T = \mathbb{1} \quad \Leftrightarrow \quad R^T = R^{-1} \tag{8}$$

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

$$\varepsilon_{ijk} = \begin{cases} 1, & (i,j,k) = (1,2,3),(2,3,1),(3,1,2) \\ -1, & (i,j,k) = (3,2,1),(2,1,3),(1,3,2) \\ 0, & \text{otherwise} \end{cases} \tag{9}$$

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

$$\boldsymbol{c} = \boldsymbol{a} \times \boldsymbol{b} \quad \Leftrightarrow \quad c_i = \varepsilon_{ijk} a_j b_k \tag{10}$$

A useful identity involving the contraction of two alternating tensors is

$$\varepsilon_{ijk}\varepsilon_{klm} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl} \tag{11}$$

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

$$\begin{aligned} [\boldsymbol{a} \times (\boldsymbol{b} \times \boldsymbol{c})]_i &= \varepsilon_{ijk} a_j (\boldsymbol{b} \times \boldsymbol{c})_k = \varepsilon_{ijk} a_j \varepsilon_{klm} b_l c_m \\ &= (\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}) a_j b_l c_m = (a_j c_j) b_i - (a_j b_j) c_i \\ &= (\boldsymbol{a} \cdot \boldsymbol{c})[\boldsymbol{b}]_i - (\boldsymbol{a} \cdot \boldsymbol{b})[\boldsymbol{c}]_i \end{aligned} \tag{12}$$

1.2.4 Eigenvalues, Eigenvectors and Diagonalization

An eigenvalue equation takes the form

$$\mathbf{A}\boldsymbol{x} = \lambda \boldsymbol{x} \quad \Leftrightarrow \quad A_{ij} x_j = \lambda x_i \tag{13}$$

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

$$(A_{ij} - \lambda \delta_{ij}) x_j = 0 \tag{14}$$

which has non-trivial solutions ($\boldsymbol{x} \neq 0$) if

$$\det(\mathbf{A} - \lambda \mathbb{1}) = 0 \tag{15}$$

If $\mathbf{A}$ is Hermitian, then λ is real. There are n of them $\{\lambda_1, \cdots, \lambda_n\}$, for each one there exists

$$A_{ij} e_j^{(a)} = \lambda_a e_i^{(a)} \tag{16}$$

The eigenvectors $\{\boldsymbol{e}^{(a)}\}$ form an $n \times n$ matrix $\mathbf{M} = \begin{pmatrix} \boldsymbol{e}^{(1)} & \boldsymbol{e}^{(2)} & \cdots & \boldsymbol{e}^{(n)} \end{pmatrix}$. $\mathbf{M}$ is unitary and

$$\mathbf{M}^\dagger \mathbf{A} \mathbf{M} = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix} \tag{17}$$

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.

$$J_i = \sigma_{ij} E_j \tag{18}$$

1.4 Transformations under Rotations

The two sets of components of $\boldsymbol{x}$ are related by an orthogonal matrix $\mathbf{L}$ and the determinant $\det(\mathbf{L}) = 1$

$$x'_i = L_{ij} x_j \tag{19}$$

Recall that orthogonality means

$$L_{ij} L_{ik} = L_{ji} L_{ki} = \delta_{jk} \tag{20}$$

The set of all such matrices forms SO(3) group. Under such a rotation/coordinate transformation, the basis transforms according to

$$\boldsymbol{e}'^{(i)} = L_{ij} \boldsymbol{e}^{(j)} \quad \Leftrightarrow \quad \boldsymbol{e}^{(i)} = L_{ji} \boldsymbol{e}'^{(j)} \tag{21}$$

Definition.

1. *A scalar $\phi(x)$ transforms under a rotation*

$$\phi(x) \to \phi'(x') = \phi(x) \tag{22}$$

2. *A vector $v_i(x)$ transforms under a rotation*

$$v_i(x) \to v'_i(x') = L_{ij} v_j(x) \tag{23}$$

3. *A rank 2 tensor transforms under a rotation*

$$T_{ij}(x) \to T'_{ij}(x') = L_{il} L_{jm} T_{lm}(x) \tag{24}$$

For higher rank tensor,

$$\boxed{T'_{ijk\cdots}(x') = L_{ip} L_{jq} L_{kr} \cdots T_{pqr\cdots}(x)} \tag{25}$$

this equation also gives the definition of a tensor.

1.5 Tensor Calculus

First we define the three direction derivatives

$$\boldsymbol{\nabla} = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}\right) \tag{26}$$

here $\partial/\partial x_i = \partial_i = \nabla_i$.

- The **gradient** of ϕ is a vector if ϕ is a scalar.

$$[\boldsymbol{\nabla}\phi]_i = \partial_i \phi \tag{27}$$

  The gradient transforms under rotations

$$\partial_i \phi(x) \to \partial_i' \phi'(x') = \frac{\partial}{\partial x_i'}\phi(x) = \frac{\partial x_p}{\partial x_i'}\frac{\partial}{\partial x_p}\phi(x) = L_{ip}\partial_p \phi(x) \tag{28}$$

  where $L_{ip} = \partial_p/\partial_i'$.

- The **divergence** of $\boldsymbol{F}$ is a scalar.

$$\boldsymbol{\nabla} \cdot \boldsymbol{F} = \partial_i F_i \tag{29}$$

- The **curl** of $\boldsymbol{F}$ is a vector.

$$(\boldsymbol{\nabla} \times \boldsymbol{F})_i = \varepsilon_{ijk}\partial_j F_k \tag{30}$$

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

$$\mathcal{L}_x[y(x)] = \left[\frac{\mathrm{d}}{\mathrm{d}x^2} + p(x)\frac{\mathrm{d}}{\mathrm{d}x} + q(x)\right] y(x) = f(x) \tag{31}$$

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**.

2.2 Variation of Parameters

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

$$y(x) = ay_1(x) + by_2(x) \tag{32}$$

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

$$y(x) = ay_1(x) + by_2(x) + y_0(x) \tag{33}$$

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

Ansatz. We assume that the particular integral of ODE is given by

$$y_0(x) = u(x)y_1(x) + v(x)y_2(x) \tag{34}$$

If $u(x)$ and $v(x)$ are constants, then $y_0(x)$ just a solution of the homogeneous equation. To simplify the calculation, therefore, we will vary these parameters subject to the constraint

$$\boxed{u'y_1 + v'y_2 = 0} \tag{35}$$

Rewrite the ODE

$$\begin{aligned}\mathcal{L}_x[y_0(x)] =& u''y_1 + 2u'y_1' + uy_1'' + v''y_2 + 2v'y_2' + vy_2'' \\ &+ p(u'y_1 + uy_1' + v'y_2 + vy_2') + q(uy_1 + vy_2) \\ =& u(y_1'' + py_1' + qy_1) + v(y_2'' + py_2' + qy_2) \\ &+ u''y_1 + 2u'y_1' + v''y_2 + 2v'y_2' + p(u'y_1 + v'y_2) \\ =& u''y_1 + 2u'y_1' + v''y_2 + 2v'y_2' \\ =& u'y_1' + v'y_2' = f\end{aligned} \tag{36}$$

gives

$$\boxed{u'y_1' + v'y_2' = f} \tag{37}$$

So we have

$$\begin{cases} u'y_1 + v'y_2 = 0 \\ u'y_1' + v'y_2' = f \end{cases} \quad \Rightarrow \quad \begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix} \begin{pmatrix} u' \\ v' \end{pmatrix} = \mathbf{M} \begin{pmatrix} u' \\ v' \end{pmatrix} = \begin{pmatrix} 0 \\ f \end{pmatrix} \tag{38}$$

then

$$\begin{pmatrix} u' \\ v' \end{pmatrix} = \mathbf{M}^{-1} \begin{pmatrix} 0 \\ f \end{pmatrix} = \frac{1}{W(x)} \begin{pmatrix} y_2' & -y_2 \\ -y_1' & y_1' \end{pmatrix} \begin{pmatrix} 0 \\ f \end{pmatrix} \tag{39}$$

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

$$W(x) = \det(\mathbf{M}) = y_1 y_2' - y_2 y_1' \tag{40}$$

So the solutions are

$$u'(x) = -\frac{y_2(x) f(x)}{W(x)}, \qquad v'(x) = \frac{y_1(x) f(x)}{W(x)} \tag{41}$$

2.2.1 Homogeneous Initial Conditions

The boundary conditions $y(\alpha) = y'(\alpha) = 0$ are called *homogeneous initial conditions*. Integrating eqn.(41) gives

$$u(x) = -\int_\alpha^x \mathrm{d}\tilde{x} \frac{y_2(\tilde{x}) f(\tilde{x})}{W(\tilde{x})}, \qquad v(x) = \int_\alpha^x \mathrm{d}\tilde{x} \frac{y_1(\tilde{x}) f(\tilde{x})}{W(\tilde{x})} \tag{42}$$

then

$$y_0(x) = u(x) y_1(x) + v(x) y_2(x) = \int_\alpha^x \mathrm{d}\tilde{x} \frac{y_1(\tilde{x}) y_2(x) - y_2(\tilde{x}) y_1(x)}{W(\tilde{x})} f(\tilde{x}) \tag{43}$$

satisfies $y_0(\alpha) = y_0'(\alpha) = 0$.

$$\begin{aligned} y_0(x) &= \int_\alpha^x \mathrm{d}\tilde{x} \frac{y_1(\tilde{x}) y_2(x) - y_2(\tilde{x}) y_1(x)}{W(\tilde{x})} f(\tilde{x}) + \int_x^\beta \mathrm{d}\tilde{x} \cdot 0 \\ &= \int_\alpha^\beta G(x, \tilde{x}) f(\tilde{x}) \mathrm{d}\tilde{x} \end{aligned} \tag{44}$$

where we have defined the *Green Function*

$$G(x, \tilde{x}) = \begin{cases} 0, & x < \tilde{x} \\ \frac{y_1(\tilde{x}) y_2(x) - y_2(\tilde{x}) y_1(x)}{W(\tilde{x})}, & x > \tilde{x} \end{cases} \tag{45}$$

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

$$Y(x) = y(x) - g(x) \tag{46}$$

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

$$F(x) = f(x) - \mathcal{L}_x g(x) = f(x) - g''(x) - p(x) g'(x) - q(x) g(x) \tag{47}$$

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

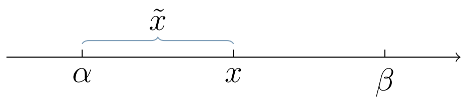

Figure 1: The range of variable x in the problem is $x \in [\alpha, \beta]$.

2.2.3 Homogeneous Two-Point Boundary Conditions

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

$$y(x) = \int_\alpha^x \mathrm{d}\tilde{x} \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) + ay_1(x) + by_2(x) \tag{48}$$

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

$$y(\alpha) = by_2(\alpha) = 0 \quad \Rightarrow \quad b = 0 \tag{49}$$

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

$$y(\beta) = -\int_\alpha^\beta \mathrm{d}\tilde{x} \frac{y_1(\beta)y_2(\tilde{x})}{W(\tilde{x})} f(\tilde{x}) + ay_1(\beta) = 0 \quad \Rightarrow \quad a = \int_\alpha^\beta \mathrm{d}\tilde{x} \frac{y_2(\tilde{x})}{W(\tilde{x})} f(\tilde{x}) \tag{50}$$

which may be substituted into the solution eqn.(48) to give

$$\begin{aligned} y(x) &= \int_\alpha^x \mathrm{d}\tilde{x} \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) + \int_\alpha^\beta \mathrm{d}\tilde{x} \frac{y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) \\ &= \int_\alpha^x \mathrm{d}\tilde{x} \frac{y_1(\tilde{x})y_2(x)}{W(\tilde{x})} f(\tilde{x}) + \int_x^\beta \mathrm{d}\tilde{x} \frac{y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) \\ &= \int_\alpha^\beta \mathrm{d}\tilde{x} G(x, \tilde{x}) f(\tilde{x}) \end{aligned} \tag{51}$$

where we have defined the *Green Function*

$$G(x, \tilde{x}) = \begin{cases} \frac{y_1(\tilde{x})y_2(x)}{W(\tilde{x})}, & \alpha \le \tilde{x} < x \\ \frac{y_2(\tilde{x})y_1(x)}{W(\tilde{x})}, & x < \tilde{x} \le \beta \end{cases} \tag{52}$$

2.3 Properties of Green Functions

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 $x \neq \tilde{x}$
$$\mathcal{L}_x[G(x, \tilde{x})] = 0 \tag{53}$$
2. $G(x, \tilde{x})$ is continuous at $x = \tilde{x}$
$$\lim_{x \to \tilde{x}_-} G(x, \tilde{x}) = \lim_{x \to \tilde{x}_+} G(x, \tilde{x}) \tag{54}$$
3. $\frac{\partial}{\partial x} G(x, \tilde{x})$ has a unit discontinuity at $x = \tilde{x}$
$$\lim_{x \to \tilde{x}_+} \frac{\partial G(x, \tilde{x})}{\partial x} = 1 + \lim_{x \to \tilde{x}_-} \frac{\partial G(x, \tilde{x})}{\partial x} \tag{55}$$

2.4 Green Function More Generally

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

$$\boxed{\mathcal{L}_x[G(x, \tilde{x})] = \delta(x - \tilde{x})} \tag{56}$$

$\delta(x)$ 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.(56), then so does $G(x, \tilde{x}) + Y(x)$, where $\mathcal{L}_x[Y(x)] = 0$. If we impose 2 boundary conditions on the Green function then it becomes unique for those boundary conditions.

Now define

$$\boxed{y_0(x) = \int_\alpha^\beta \mathrm{d}\tilde{x} G(x, \tilde{x}) f(\tilde{x})} \tag{57}$$

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.

$$\mathcal{L}_x[y_0] = \int_\alpha^\beta \mathrm{d}\tilde{x} \mathcal{L}_x[G(x, \tilde{x})] f(\tilde{x}) = \int_\alpha^\beta \mathrm{d}\tilde{x} \delta(x - \tilde{x}) f(\tilde{x}) = f(x) \tag{58}$$

$f(x)$ 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

$$y_0(x) = \int_\alpha^\beta \mathrm{d}\tilde{x} G(x, \tilde{x}) f(\tilde{x}) \tag{59}$$

This is called *linear response*.

2.4.1 Homogeneous Initial Conditions

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

$$y(x) = \int_\alpha^\beta \mathrm{d}\tilde{x} G(x, \tilde{x}) f(\tilde{x}) \tag{60}$$

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 $x < \tilde{x}$
$$G(x,\tilde{x}) = 0 \tag{61}$$

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 $y_2(x)$
$$G(x,\tilde{x}) = A(\tilde{x})y_1(x) + B(\tilde{x})y_2(x) \tag{62}$$
We can find A and B by using the properties of G:

   (i) G is continuous at $x = \tilde{x}$
$$A(\tilde{x})y_1(\tilde{x}) + B(\tilde{x})y_2(\tilde{x}) = 0 \tag{63}$$

   (ii) G' has a unit discontinuity at $x = \tilde{x}$
$$A(\tilde{x})y_1'(\tilde{x}) + B(\tilde{x})y_2'(\tilde{x}) = 1 \tag{64}$$

   The solution is
$$A(\tilde{x}) = -\frac{y_x(\tilde{x})}{W(\tilde{x})}, \qquad B(\tilde{x}) = \frac{y_1(\tilde{x})}{W(\tilde{x})} \tag{65}$$
   where W is the Wronskian of y_1 and y_2.

So we have
$$G(x,\tilde{x}) = \begin{cases} 0, & x < \tilde{x} \\ \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})}, & x > \tilde{x} \end{cases} \tag{66}$$
which agrees with that calculated before.

2.4.2 Homogeneous Two-Point Boundary Conditions

The boundary conditions are $y(\alpha) = y(\beta) = 0$. The Green Function should satisfies
$$G(\alpha,\tilde{x}) = G(\beta,\tilde{x}) = 0 \tag{67}$$
We assume y_1 and y_2 are linear independent solutions of homogeneous equation, and we choose $y_1(\alpha) = y_2(\beta) = 0$.
$$G(x,\tilde{x}) = \begin{cases} A(\tilde{x})y_1(x) + B(\tilde{x})y_2(x), & \alpha < x < \tilde{x} \\ C(\tilde{x})y_1(x) + D(\tilde{x})y_2(x), & \tilde{x} < x < \beta \end{cases} \tag{68}$$

1. Boundary conditions: $G(\alpha,\tilde{x}) = G(\beta,\tilde{x}) = 0$
$$A(\tilde{x})y_1(\alpha) + B(\tilde{x})y_2(\alpha) = B(\tilde{x})y_2(\alpha) = 0 \quad \Rightarrow \quad B(\tilde{x}) = 0 \tag{69}$$
$$C(\tilde{x})y_1(\beta) + D(\tilde{x})y_2(\beta) = C(\tilde{x})y_1(\beta) = 0 \quad \Rightarrow \quad C(\tilde{x}) = 0 \tag{70}$$
so we have
$$G(x,\tilde{x}) = \begin{cases} A(\tilde{x})y_1(x), & \alpha < x < \tilde{x} \\ D(\tilde{x})y_2(x), & \tilde{x} < x < \beta \end{cases} \tag{71}$$

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

$$A(\tilde{x})y_1(\tilde{x}) - D(\tilde{x})y_2(\tilde{x}) = 0 \tag{72}$$

$$A(\tilde{x})y_1'(\tilde{x}) - D(\tilde{x})y_2'(\tilde{x}) = 1 \tag{73}$$

so we have

$$A(\tilde{x}) = \frac{y_2(\tilde{x})}{W(\tilde{x})}, \qquad D(\tilde{x}) = \frac{y_1(\tilde{x})}{W(\tilde{x})} \tag{74}$$

The final result

$$G(x,\tilde{x}) = \begin{cases} \frac{y_2(\tilde{x})y_1(x)}{W(\tilde{x})}, & \alpha < x < \tilde{x} \\ \frac{y_1(\tilde{x})y_2(x)}{W(\tilde{x})}, & \tilde{x} < x < \beta \end{cases} \tag{75}$$

which agrees with that calculated before.

2.4.3 Higher Dimensions, More Variables

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

$$\mathcal{L}[y] = f(x_1, x_2, x_3) \tag{76}$$

and

$$\mathcal{L}[G(\boldsymbol{x}, \tilde{\boldsymbol{x}})] = \delta^{(3)}(\boldsymbol{x} - \tilde{\boldsymbol{x}}) = \delta(x_1 - \tilde{x}_1)\delta(x_2 - \tilde{x}_2)\delta(x_3 - \tilde{x}_3) \tag{77}$$

Let R be a three-dimension region in three-dimension Euclidean space

$$\int_R \mathrm{d}\tilde{\boldsymbol{x}} \delta^{(3)}(\boldsymbol{x} - \tilde{\boldsymbol{x}}) f(\tilde{\boldsymbol{x}}) = \begin{cases} f(\boldsymbol{x}), & \boldsymbol{x} \in R \\ 0, & \boldsymbol{x} \notin R \end{cases} \tag{78}$$

Example. The most famous example is

$$\mathcal{L} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \nabla^2 \tag{79}$$

and the Green function satisfies

$$\nabla^2 G(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = \delta(\boldsymbol{x} - \tilde{\boldsymbol{x}}) \tag{80}$$

Consider the Poisson equation for the scalar gravitational potential $\phi(\boldsymbol{x})$ in terms of the scalar mass density $\rho(\boldsymbol{x})$

$$\nabla^2 \phi(\boldsymbol{x}) = 2\pi G \rho \tag{81}$$

The Green function for the Poisson equation that satisfying the boundary condition $G(\boldsymbol{x}, \tilde{\boldsymbol{x}}) \to 0$ as $|\boldsymbol{x}| \to \infty$ is

$$G(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = -\frac{1}{4\pi|\boldsymbol{x} - \tilde{\boldsymbol{x}}|} \tag{82}$$

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
$$\langle f, g\rangle = \int_a^b f^*(x)g(x)\mathrm{d}x \tag{83}$$
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
$$f(x) = \sum_{i=1}^{\infty} f_i y_i(x), \quad f_i \in \mathbb{C} \tag{84}$$
Then we have
$$\langle y_k, f\rangle = \langle y_k, \sum_{i=1}^{\infty} f_i y_i\rangle = \sum_{i=1}^{\infty} f_i\langle y_k, y_i\rangle = \sum_{i=1}^{\infty} f_i\delta_{ik} = f_k \tag{85}$$

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 the differential operator
$$\boxed{\mathcal{L} = -\frac{\mathrm{d}}{\mathrm{d}x}\left[\rho(x)\frac{\mathrm{d}}{\mathrm{d}x}\right] + \sigma(x)} \tag{86}$$
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].
$$\mathcal{L}y = -\frac{\mathrm{d}}{\mathrm{d}x}\left(\rho\frac{\mathrm{d}y}{\mathrm{d}x}\right) + \sigma y = -(\rho y')' + \sigma y \tag{87}$$

Definition. *A second order linear differential operator $\mathcal{D}$ is self-adjoint on Hilbert space $\mathcal{H}$ if*
$$\boxed{\langle u, \mathcal{D}v\rangle = \langle v, \mathcal{D}u\rangle^* = \langle\mathcal{D}u, v\rangle, \quad \forall u, v \in \mathcal{H}} \tag{88}$$

[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.

Compare with the definition of a Hermitian matrix $\mathbf{M} : M_{ij} = M_{ji}^*$.

Consider $\mathcal{L}$ as in self-adjoint form,

$$\begin{aligned}\langle u, \mathcal{L}v\rangle &= \int_a^b u^* \left[-(\rho v')' + \sigma v\right] \mathrm{d}x \\ &= - u^* \rho v' \Big|_a^b + \int_a^b \left(u^{*\prime} \rho v' + u^* \sigma v\right) \mathrm{d}x \\ &= - u^* \rho v' \Big|_a^b + u^{*\prime} \rho v \Big|_a^b + \int_a^b \left(-(u^{*\prime}\rho)' v + u^* \sigma v\right) \mathrm{d}x \\ &= (-u^* \rho v' + u^{*\prime} \rho v)\Big|_a^b + \int_a^b \left(-(u^{*\prime}\rho)' + u^* \sigma\right) v \mathrm{d}x \\ &= (-u^* \rho v' + u^{*\prime} \rho v)\Big|_a^b + \left[\int_a^b \left(-(u'\rho)' + u\sigma\right) v^* \mathrm{d}x\right]^* \\ &= (-u^* \rho v' + u^{*\prime} \rho v)\Big|_a^b + \langle v, \mathcal{L}u\rangle^*\end{aligned} \tag{89}$$

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

$$\rho(b)u^{*\prime}(b)v(b) - \rho(b)u^*(b)v'(b) - \rho(a)u^{*\prime}(a)v(a) + \rho(a)u^*(a)v'(a) = 0 \tag{90}$$

Clearly something to do with the 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

$$\begin{cases} C_1 u(a) + C_2 u'(a) = 0 \\ D_1 u(b) + D_2 u'(b) = 0 \end{cases} \tag{91}$$

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

3.1.2 Weight Functions

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

$$\tilde{\mathcal{L}} = -\frac{\mathrm{d}}{\mathrm{d}x}\left(A(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) - B(x)\frac{\mathrm{d}}{\mathrm{d}x} + C(x) \tag{92}$$

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.*

$$w(x)\left[-(Ay')' - By' + Cy\right] = -(\rho y')' + \sigma y \tag{93}$$

rearranging this

$$-w(Ay')' - Bwy' + Cwy = -(\rho y')' + \sigma y \tag{94}$$

so we have

$$\begin{cases} Awy'' = \rho y'' \\ A'wy' - Bwy' = \rho' y' \\ Cwy = \sigma y \end{cases} \tag{95}$$

then

$$\frac{w'}{w} = \frac{B}{A}, \qquad Aw = \rho, \qquad Cw = \sigma \tag{96}$$

We choose $w(x)$ such that

$$w(x) = \exp\left[\int_a^x \frac{B(\tilde{x})}{A(\tilde{x})}\mathrm{d}\tilde{x}\right] \tag{97}$$

where $w(a) = 1$.

Definition. *The inner product with weight* $w \in \mathbb{R}$

$$\langle f, g\rangle_w = \langle f, wg\rangle = \int_a^b f^*(x)w(x)g(x)\mathrm{d}x = \langle wf, g\rangle \tag{98}$$

3.1.3 Eigenfunctions and Eigenvalues

Consider the inhomogeneous eigenfunction equation

$$\tilde{\mathcal{L}}y = \lambda y \tag{99}$$

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

$$\boxed{\mathcal{L}y = \lambda wy} \tag{100}$$

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

1. The eigenvalues λ are real.
2. The eigenfunctions y with distinct eigenvalues are orthogonal.

Proof. 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

$$\langle y_i, \mathcal{L}y_j\rangle = \langle y_j, \mathcal{L}y_i\rangle^* = \lambda_i^*\langle y_j, \omega y_i\rangle^* = \lambda_i^*\langle y_i, \omega y_j\rangle = \lambda_i^*\langle y_i, y_j\rangle_w \tag{101}$$

$$\langle y_i, \mathcal{L}y_j\rangle = \lambda_j\langle y_i, wy_j\rangle = \lambda_j\langle y_i, y_j\rangle_w \tag{102}$$

Compare the two equations, we find

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

- For $i = j$ we have
$$(\lambda_i^* - \lambda_i)\|y_i\|_w^2 = 0 \tag{104}$$
so, if we have non-zero eigenfunctions, then $\lambda_i^* = \lambda_i$, *i.e.*, the eigenvalues are real.

- For $i \neq j$ we have
$$(\lambda_i - \lambda_j)\langle y_i, y_j\rangle_w = 0 \tag{105}$$
so, if we are considering distinct eigenvalues, then $\langle y_i, y_j\rangle_w = 0$, *i.e.*, the eigenfunctions are orthogonal with weight $w(x)$.

□

3.1.4 Eigenfunction Expansions

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
$$g(x) = \sum_n g_n f_n(x), \quad g_n \in \mathbb{C} \tag{106}$$
where
$$g_n = \langle f_n, g\rangle_\omega = \int_a^b f_n^*(x) w(x) g(x) \mathrm{d}x \tag{107}$$
Substituting into the expansion we find
$$\begin{aligned} g(x) &= \sum_n \int_a^b \mathrm{d}\tilde{x}\, [f_n^*(\tilde{x}) w(\tilde{x}) g(\tilde{x})]\, f_n(x) \\ &= \int_a^b \mathrm{d}\tilde{x} g(\tilde{x}) \left[w(\tilde{x}) \sum_n f_n(x) f_n^*(\tilde{x}) \right] \\ &= \int_a^b \mathrm{d}\tilde{x} \delta(x - \tilde{x}) g(\tilde{x}) \end{aligned} \tag{108}$$
where
$$\boxed{\delta(x - \tilde{x}) = w(\tilde{x}) \sum_n f_n(\tilde{x}) f_n^*(\tilde{x})} \tag{109}$$
Let $u \in \mathcal{H}$, consider the expression
$$\begin{aligned} \int_a^b |u|^2 \omega \mathrm{d}x =& \langle u, u\rangle_w = \langle \sum_n u_n f_n(x), \sum_m u_m f_m(x)\rangle_w \\ =& \sum_{n,m} u_n^* u_m \langle f_n, f_m\rangle_w = \sum_{n,m} u_n^* u_m \delta_{nm} = \sum_n |u_n|^2 \end{aligned} \tag{110}$$
which is *Parseval's identity* in the case with a weight function $w(x)$
$$\langle u, u\rangle_w = \sum_n |u_n|^2 \tag{111}$$

3.1.5 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

$$\boxed{G(x,\tilde{x}) = \sum_n \frac{y_n(x)y_n^*(\tilde{x})}{\lambda_n}, \qquad \lambda_n \neq 0} \tag{112}$$

Proof.

$$\begin{aligned}\mathcal{L}_x[G(x,\tilde{x})] &= \sum_n \frac{\mathcal{L}_x[y_n(x)]y_n^*(\tilde{x})}{\lambda_n} \\ &= \sum_n w(x)y_n(x)y_n^*(\tilde{x}) \\ &= \frac{\omega(x)}{\omega(\tilde{x})}\left[\omega(\tilde{x})\sum_n y_n(x)y_n^*(\tilde{x})\right] \\ &= \delta(x-\tilde{x})\end{aligned} \tag{113}$$

□

3.1.6 Eigenfunction Expansions for Solving ODEs

As an example, consider the differential equation

$$\mathcal{L}y - \nu y = f \tag{114}$$

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

$$y(x) = \sum_n a_n y_n(x), \qquad f(x) = \sum_n f_n y_n(x) \tag{115}$$

Substituting into the original equation, we find

$$\mathcal{L}\sum_n a_n y_n - \nu \sum_n a_n y_n = \sum_n (a_n\lambda_n - \nu a_n)y_n = \sum_n f_n y_n \tag{116}$$

So that

$$a_n = \frac{f_n}{\lambda_n - \nu}, \qquad (\lambda_n \neq \nu) \tag{117}$$

so that the solution is given by

$$\begin{aligned}y(x) &= \sum_n \frac{f_n}{\lambda_n - \nu} y_n(x) = \sum_n \frac{\langle y_n, f\rangle}{\lambda_n - \nu} y_n(x) \\ &= \int_a^b \mathrm{d}x' \sum_n \frac{y_n(x)y_n^*(x')}{\lambda_n - \nu} f(x') \\ &= \int_a^b \mathrm{d}x' G(x,x')f(x')\end{aligned} \tag{118}$$

hence the Green function of the problem as

$$G(x, x') = \sum_n \frac{y_n(x) y_n^*(x')}{\lambda_n - \nu} \tag{119}$$

Note that if $\nu = \lambda_n$, for any n, then there is no Green function.

3.2 Legendre Polynomials

3.2.1 Examples

Example. The two examples differ only by boundary conditions.

(1) Let

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

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

$$-y_n'' = \lambda_n y_n \tag{121}$$

and the eigenfunctions and the corresponding eigenvalues are

$$y_n = \sin\left(\frac{n}{2R} x\right), \qquad \lambda_n = \left(\frac{n}{2R}\right)^2, \qquad n = 1, 2, 3, \cdots \tag{122}$$

(2) Let

$$\mathcal{L} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \qquad x \in [0, 2\pi R] \tag{123}$$

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

$$-y_m'' = \lambda_m y_m \tag{124}$$

and the eigenfunctions and the corresponding eigenvalues are

$$y_m = \exp\left(i \frac{m}{R} x\right), \qquad \lambda_m = \left(\frac{m}{2R}\right)^2, \qquad m \in \mathbb{Z} \tag{125}$$

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

3.2.2 Legendre's Equation

Legendre's equation

$$(1 - x^2) y'' - 2xy' + l(l+1)y = 0 \quad \text{with} \quad x \in [-1, 1] \tag{126}$$

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

$$\boxed{-\frac{\mathrm{d}}{\mathrm{d}x}\left[(1 - x^2) y'\right] = l(l+1) y} \tag{127}$$

or

$$\mathcal{L}y = l(l+1)y \tag{128}$$

where

$$\mathcal{L} = -\frac{\mathrm{d}}{\mathrm{d}x}\left[(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}\right] \tag{129}$$

is self-adjoint on a Hilbert space of functions that are finite at ± 1. Assume that eigenfunctions of eqn.(127) are polynomials

$$y_n(x) = x^{m_n} + a_{m_n-1}x^{m_n-1} + \cdots + a_1 x + a_0 \tag{130}$$

Substituting the polynomial solution y_n into eqn.(127), then thinking about equation coefficients of partial of x. The highest power m_n satisfies the relation

$$m_n(m_n+1) = \lambda \tag{131}$$

So eigenvalues take form

$$\lambda = l(l+1), \qquad l \in \mathbb{N} \tag{132}$$

and can label eigenfunctions by l

- $l = 0$, $y_0(x) = 1$
- $l = 1$, $y_1(x) = x + a_0$
- $l = 2$, $y_2(x) = x^2 + a_1 x + a_0$

They are orthogonal with each other

$$\int_{-1}^{1} y_l^*(x) y_{l'}(x) = \delta_{ll'} \tag{133}$$

3.3 Spherical Harmonics

Laplace's equation in spherical coordinates is given by

$$\nabla^2 f(r,\theta,\phi) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin\theta}\frac{\partial^2 f}{\partial\phi^2} \tag{134}$$

Ansatz

$$f(r,\theta,\phi) = r^l \mathrm{e}^{im\phi}\Theta(\theta) \tag{135}$$

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

$$l(l+1)\mathrm{e}^{im\phi}\Theta(\theta) + \frac{\mathrm{e}^{im\phi}}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) - \frac{\Theta}{\sin\theta}m^2\mathrm{e}^{im\phi} = 0 \tag{136}$$

Rearrange this, we have

$$\sin^2\theta\, l(l+1) + \frac{\sin\theta}{\Theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) = m^2 \tag{137}$$

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

$$\frac{\mathrm{d}}{\mathrm{d}\theta} = \frac{\mathrm{d}}{\mathrm{d}u}\frac{\mathrm{d}u}{\mathrm{d}\theta} = -\sin\theta\frac{\mathrm{d}}{\mathrm{d}u} \tag{138}$$

Then the equation becomes self-adjoint form

$$-[(1-u^2)P']' + \frac{m^2}{1-u^2}P = l(l+1)P \tag{139}$$

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 $[-1, 1]$. Check the orthogonality

$$\int_{-1}^{1} P_l^m(u)P_{l'}^m(u)\mathrm{d}u = \frac{2(l+m)!}{(2l+1)(l-m)}\delta_{ll'} \tag{140}$$

Similarly, the equation can be expressed as

$$-[(1-u^2)P']' - l(l+1)P = -\frac{m^2}{1-u^2}P \tag{141}$$

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

$$\int_{-1}^{1} \frac{P_l^m(u)P_l^{m'}(u)}{1-u^2}\mathrm{d}u = \frac{(l+m)!}{m(l-m)}\delta_{mm'} \tag{142}$$

Finally we get

$$Y_l^m = (-1)^m\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)\mathrm{e}^{im\phi}, \quad l \in \mathbb{N},\ -l \le m \le l \tag{143}$$

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

$$\delta_{ll'}\delta_{mm'} = \int_0^{2\pi}\int_0^{\pi} Y_l^m(\theta,\phi)Y_{l'}^{m'}(\theta,\phi)\sin\theta\mathrm{d}\theta\mathrm{d}\phi \tag{144}$$

So any function f can be expressed as

$$f(\theta,\phi) = \sum_l \sum_{m=-l}^{l} f_{lm}Y_l^m(\theta,\phi) \tag{145}$$

where

$$f_{lm} = \int_{\mathbf{S}^2} Y_l^{*m} f\mathrm{d}\Omega \tag{146}$$

4 Integral Transforms

4.1 Fourier Series

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

$$f(x) = \sum_{n=-\infty}^{\infty} f_n y_n(x), \qquad f_n \in \mathbb{C} \tag{147}$$

We choose the Fourier basis

$$y_n(x) = \frac{1}{\sqrt{2\pi R}} \mathrm{e}^{inx/R} \tag{148}$$

with the orthogonality

$$\langle y_n, y_m \rangle = \int_0^{2\pi R} y_n^* y_m \mathrm{d}x = \delta_{nm} \tag{149}$$

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

$$\begin{aligned} f_n &= \int_{-\pi R}^{\pi R} y_n^*(x) f(x) \mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi R}} \int_{-\pi R}^{\pi R} \mathrm{e}^{-inx/R} f(x) \mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi R}} \int_{-\pi R}^{\pi R} \mathrm{e}^{-ik_n x} f(x) \mathrm{d}x \end{aligned} \tag{150}$$

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

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} f(x) \mathrm{d}x \tag{151}$$

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

4.2 Fourier Transforms

4.2.1 Definition and Notation

Definition. *The Fourier transform is defined as*

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

The inverse Fourier transform is defined as

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

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

$$\mathcal{F}^{-1}[\mathcal{F}[f]] = f \quad \Rightarrow \quad \mathcal{F}^{-1}\mathcal{F} = \mathbb{1} \tag{154}$$

4.2.2 Dirac Delta-Function

$$
\begin{aligned}
f(x) =& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) \mathrm{e}^{ikx} \mathrm{d}k \\
=& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x') \mathrm{e}^{-ikx'} \mathrm{d}x' \right] \mathrm{e}^{ikx} \mathrm{d}k \\
=& \int_{-\infty}^{\infty} f(x') \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{ik(x-x')} \mathrm{d}k \right] \mathrm{d}x' \\
=& \int_{-\infty}^{\infty} f(x') \delta(x-x') \mathrm{d}x'
\end{aligned}
\tag{155}
$$

where we have defined the *Dirac delta-function*

$$
\boxed{\delta(x-x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{ik(x-x')} \mathrm{d}k}
\tag{156}
$$

4.2.3 Properties of the Fourier Transform

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

$$
\tilde{f}^*(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-i(-k)x} f^*(x) \mathrm{d}x = \tilde{f}(-k)
\tag{157}
$$

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

$$
\tilde{f}^*(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-iky} f(-y) \mathrm{d}(-y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-iky} f(y) \mathrm{d}y = \tilde{f}(k)
\tag{158}
$$

□

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

Proof. Define $y = -x$, then

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

□

2. Differentiation

$$
\mathcal{F}[f^{(n)}(x)] = (ik)^n \tilde{f}(k)
\tag{160}
$$

Proof. Consider the first order derivative

$$
\begin{aligned}
\mathcal{F}[f'(x)] =& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{-ikx} f'(x) \\
=& \frac{1}{\sqrt{2\pi}} \left[f(x) \mathrm{e}^{-ikx} \right]_{-\infty}^{\infty} - \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x f(x) (-ik) \mathrm{e}^{-ikx} \\
=& ik\tilde{f}(k)
\end{aligned}
\tag{161}
$$

Repeat the process so we can prove the relation. □

3. Multiplication by x

$$\mathcal{F}[xf(x)] = i\frac{\mathrm{d}}{\mathrm{d}x}\tilde{f}(k) \tag{162}$$

$$\mathcal{F}[x^n f(x)] = \left(i\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \tilde{f}(k) \tag{163}$$

4. Rigid shift of coordinate

$$\mathcal{F}[f(x-a)] = \mathrm{e}^{-ika}\tilde{f}(k) \tag{164}$$

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

$$\begin{aligned}\mathcal{F}[f(x-a)] =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{-ikx} f(x-a)\mathrm{d}x \\ =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{e}^{-ika}\mathrm{e}^{-ik(x-a)} f(x-a)\mathrm{d}(x-a) \\ =& \frac{1}{\sqrt{2\pi}}\mathrm{e}^{-ika}\int_{-\infty}^{\infty} \mathrm{e}^{-iky} f(y)\mathrm{d}y = \mathrm{e}^{-ika}\tilde{f}(k)\end{aligned} \tag{165}$$

□

4.2.4 Parseval's Theorem

Parseval's theorem for Fourier transforms states that

$$\boxed{\int_{-\infty}^{\infty} |f(x)|^2\mathrm{d}x = \int_{-\infty}^{\infty} |\tilde{f}(k)|^2\mathrm{d}k} \tag{166}$$

Proof.

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

□

4.2.5 Convolution Theorem

Theorem.

$$\boxed{(f * g)(x) = \int_{-\infty}^{\infty} f(y)g(x-y)\mathrm{d}y} \tag{168}$$

is the *convolution* of f and g. We claim that

1. $f * g = g * f$
2. $f * \delta = f$

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

(1) The Fourier transform of a convolution is the product of the Fourier transforms.

$$\mathcal{F}(f * g) = \sqrt{2\pi}\tilde{f}(k)\tilde{g}(k) \tag{169}$$

Proof.

$$\begin{aligned}\mathcal{F}[f * g] =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}x\mathrm{e}^{-ikx}\int_{-\infty}^{\infty} \mathrm{d}y f(y)g(x-y) \\ =& \int_{-\infty}^{\infty} \mathrm{d}y\mathrm{e}^{-iky}f(y)\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}(x-y)\mathrm{e}^{-ik(x-y)}g(x-y) \\ =& \int_{-\infty}^{\infty} \mathrm{d}y\mathrm{e}^{-iky}f(y)\tilde{g}(k) = \sqrt{2\pi}\tilde{f}(k)\tilde{g}(k)\end{aligned} \tag{170}$$

□

(2) The Fourier tranform of a product is the convolution of the Fourier transforms.

$$\mathcal{F}[f(x)g(x)] = \frac{1}{\sqrt{2\pi}}\tilde{f}(k) * \tilde{g}(k) \tag{171}$$

Proof. We start from the first form $\mathcal{F}(f * g) = \sqrt{2\pi}\tilde{f}(k)\tilde{g}(k)$

$$f * g = \mathcal{F}^{-1}[\tilde{f}(k)] * \mathcal{F}^{-1}[\tilde{g}(k)] = \sqrt{2\pi}\mathcal{F}^{-1}[\tilde{f}(k)\tilde{g}(k)] \tag{172}$$

But, as we noted above, we could have proved the convolution theorem for the inverse transform in the same way, so we can reexpress this result in terms of the forward transform. □

4.2.6 Examples of Fourier Transform

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

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

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

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{ik_0x}\mathrm{e}^{-ikx}\mathrm{d}x = \sqrt{2\pi}\delta(k-k_0) \tag{174}$$

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

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(x-x_0)\mathrm{e}^{-ikx}\mathrm{d}x = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{-ikx_0} \tag{175}$$

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

$$\begin{aligned}
\tilde{f}(k) =& \frac{1}{\sqrt{2\pi}}\frac{1}{\sigma(2\pi)^{1/4}} \int_{-\infty}^{\infty} \mathrm{e}^{-x^2/4\sigma^2}\mathrm{e}^{-ikx}\mathrm{d}x \\
=& \frac{1}{\sqrt{2\pi}}\frac{1}{\sigma(2\pi)^{1/4}} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{4\sigma^2} - ikx\right)\mathrm{d}x \\
=& \frac{1}{\sqrt{2\pi}}\frac{1}{\sigma(2\pi)^{1/4}} \int_{-\infty}^{\infty} \exp\left[-\frac{1}{4\sigma^2}\left(x+ik2\sigma\right)^2 - k^2\sigma^2\right]\mathrm{d}x \\
=& \frac{1}{\sqrt{2\pi}}\frac{1}{\sigma(2\pi)^{1/4}}\mathrm{e}^{-k^2\sigma^2} \int_{-\infty}^{\infty} \exp\left[-\frac{1}{4\sigma^2}\left(x+ik2\sigma\right)^2\right]\mathrm{d}x \\
=& \frac{1}{\sqrt{2\pi}}\frac{1}{\sigma(2\pi)^{1/4}}\mathrm{e}^{-k^2\sigma^2} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{4\sigma^2}x'^2\right)\mathrm{d}x' \\
=& \frac{\sqrt{2\sigma}}{(2\pi)^{\frac{1}{4}}}\mathrm{e}^{-k^2\sigma^2}
\end{aligned} \tag{176}$$

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

$$\begin{aligned}
\tilde{f}(k) =& \frac{1}{\sqrt{2\pi}} \int_{-a}^{a} \mathrm{e}^{-ikx}\mathrm{d}x = \frac{1}{\sqrt{2\pi}}\left[-\frac{1}{ik}\mathrm{e}^{-ikx}\right]_{-a}^{a} \\
=& \sqrt{\frac{2}{\pi}}\frac{\sin(ka)}{k} = a\sqrt{\frac{2}{\pi}}\mathrm{sinc}(ak)
\end{aligned} \tag{177}$$

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

$$h(x) = \begin{cases} 1 & |x| < \frac{a}{2} \\ 0 & |x| \geq \frac{a}{2} \end{cases} \tag{178}$$

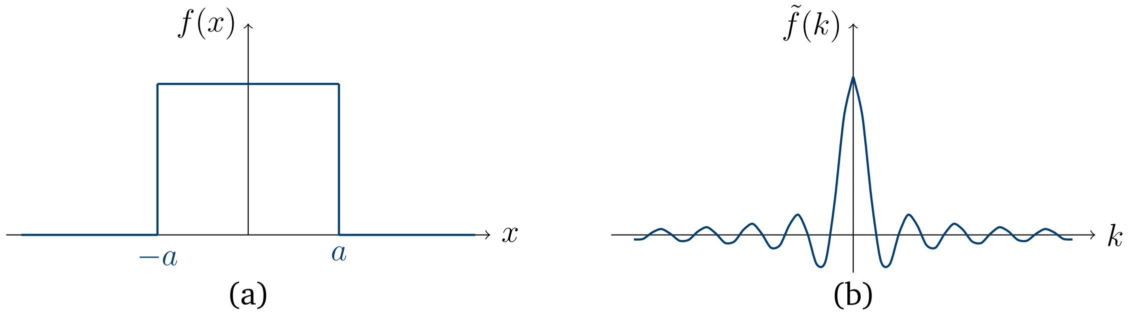

Figure 2: Top-hat function.

so we have

$$\tilde{h}(k) = \frac{a}{\sqrt{2\pi}} \mathrm{sinc}\left(\frac{ak}{2}\right) \tag{179}$$

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

$$I(x = X) = I\left(k_x = \frac{2\pi X}{\lambda D}\right) = |\tilde{h}(k_x)|^2 = \frac{a^2}{2\pi} \mathrm{sinc}^2\left(\frac{a\pi X}{2\lambda D}\right) \tag{180}$$

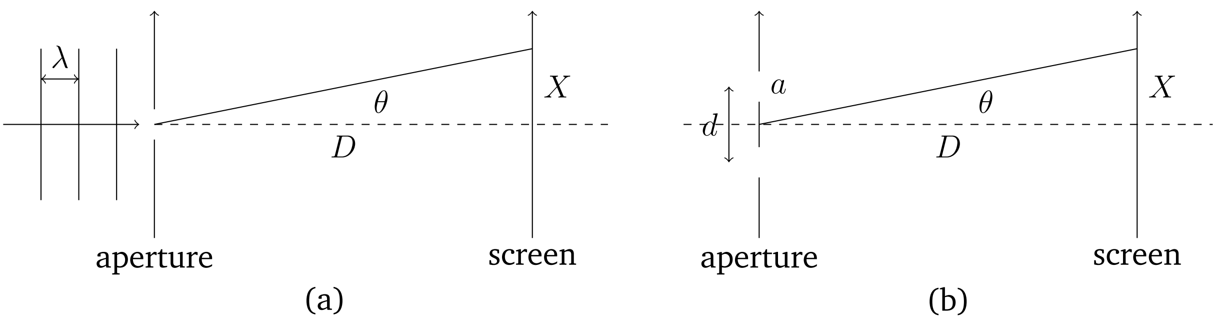

Figure 3: Geometry for Fraunhofer diffraction. (a) Diffraction through an aperture. (b) Double slit diffraction.

4.3.2 Double Slit Diffraction

The aperture function is given by

$$h(x) = f(x)g(x) \tag{181}$$

where

$$f(x) = \delta\left(x - \frac{d}{2}\right) + \delta\left(x + \frac{d}{2}\right) \tag{182}$$

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

$$\begin{aligned} \tilde{f}(k) =& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{-ikx} \left[\delta\left(x - \frac{d}{2}\right) + \delta\left(x + \frac{d}{2}\right)\right] \\ =& \frac{1}{\sqrt{2\pi}} \left(\mathrm{e}^{-ikd/2} + \mathrm{e}^{ikd/2}\right) = \sqrt{\frac{2}{\pi}} \cos\left(\frac{kd}{2}\right) \end{aligned} \tag{183}$$

so we have

$$\begin{aligned}\mathcal{F}(f*g)=&\sqrt{2\pi}\tilde{f}(k)\tilde{g}(k)\\=&\sqrt{2\pi}\sqrt{\frac{2}{\pi}}\cos\left(\frac{kd}{2}\right)\frac{a}{\sqrt{2\pi}}\text{sinc}\left(\frac{ak}{2}\right)\\=&\sqrt{\frac{2}{\pi}}a\text{sinc}\left(\frac{ak}{2}\right)\cos\left(\frac{kd}{2}\right)\end{aligned}\tag{184}$$

and the intensity on the screen is given by

$$I(k)=\frac{2a^2}{\pi}\text{sinc}^2\left(\frac{ak}{2}\right)\cos^2\left(\frac{kd}{2}\right)\tag{185}$$

4.3.3 Diffusion Equation

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

$$\frac{\partial\theta}{\partial t}=D\frac{\partial^2\theta}{\partial x^2}\tag{186}$$

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

$$\frac{\partial}{\partial t}\tilde{\theta}(k,t)=D(ik)^2\tilde{\theta}(k,t)=-Dk^2\tilde{\theta}(k,t)\tag{187}$$

the solution is

$$\tilde{\theta}(k,t)=\tilde{\theta}(k,0)\mathrm{e}^{-Dk^2t}=\mathcal{F}[\delta(x)]\mathrm{e}^{-Dk^2t}=\frac{1}{\sqrt{2\pi}}\mathrm{e}^{-Dk^2t}\tag{188}$$

So we have

$$\begin{aligned}\theta(x,t)=&\mathcal{F}^{-1}[\tilde{\theta}(k,t)]\\=&\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}k\mathrm{e}^{ikx}\mathrm{e}^{-Dk^2t}\\=&\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}k\exp\left[-Dt\left(k-\frac{ix}{2Dt}\right)^2-\frac{x^2}{4Dt}\right]\mathrm{d}k\\=&\frac{1}{2\pi}\mathrm{e}^{-x^2/4Dt}\int_{-\infty}^{\infty}e^{-Dtq^2}\mathrm{d}q\\=&\frac{1}{2\pi}\sqrt{\frac{\pi}{Dt}}\mathrm{e}^{-x^2/4Dt}\quad\left(\int_{-\infty}^{\infty}\mathrm{e}^{-\alpha x^2}\mathrm{d}x=\sqrt{\frac{\pi}{\alpha}}\right)\end{aligned}\tag{189}$$

Hence the final result

$$\theta(x,t)=\frac{1}{2\sqrt{\pi Dt}}\mathrm{e}^{-x^2/4Dt}\tag{190}$$

4.4 Laplace Transforms

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

$$\mathcal{L}[f(t)] = \hat{f}(s) = \int_0^\infty \mathrm{d}t \mathrm{e}^{-st} f(t) \tag{191}$$

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

4.4.1 Properties

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

  Proof.

$$\begin{aligned} \mathcal{L}[f'(t)] =& \int_0^\infty \mathrm{d}t \mathrm{e}^{-st} f'(t) \\ =& \mathrm{e}^{-st} f(t)\big|_0^\infty + s\int_0^\infty \mathrm{d}t \mathrm{e}^{-st} f(t) = s\hat{f}(s) - f(0) \end{aligned} \tag{192}$$

  □

  More generally, $\mathcal{L}[f^{(n)}(t)] = s^n \hat{f}(s) - s^{n-1} f(0) - s^{n-2} f'(0) - \cdots - f^{(n-1)}(0)$.

- $\mathcal{L}[t^n f(t)] = (-1)^n \frac{\mathrm{d}^n}{\mathrm{d}s^n} \hat{f}(s)$

  Proof.

$$\begin{aligned} (-1)^n \frac{\mathrm{d}^n}{\mathrm{d}s^n} \hat{f}(s) =& (-1)^n \frac{\mathrm{d}^n}{\mathrm{d}s^n} \int_0^\infty \mathrm{d}t \mathrm{e}^{-st} f(t) = (-1)^n \int_0^\infty \mathrm{d}t (-t)^n \mathrm{e}^{-st} f(t) \\ =& \int_0^\infty \mathrm{d}t \mathrm{e}^{-st} t^n f(t) = \mathcal{L}[t^n f(t)] \end{aligned} \tag{193}$$

  □

4.4.2 Examples

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

4.4.3 Convolution Theorem for Laplace Transforms

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

$$f_1 * f_2 = \int_{-\infty}^{\infty} f_1(t')f_2(t-t')\mathrm{d}t' \tag{194}$$

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

$$\boxed{f_1 * f_2 = \int_0^t f_1(t')f_2(t-t')\mathrm{d}t'} \tag{195}$$

Theorem.
The convolution theorem for Laplace transforms

$$\mathcal{L}[f_1 * f_2] = \tilde{f}_1(s)\tilde{f}_2(s) \tag{196}$$

Proof.

$$\begin{aligned}\mathcal{L}[f_1 * f_2] &= \int_0^\infty \mathrm{d}t\mathrm{e}^{-st}\int_0^t f_1(t')f_2(t-t')\mathrm{d}t' \\ &= \int_0^\infty \mathrm{d}t' f_1(t')\int_{t'}^\infty \mathrm{d}t\mathrm{e}^{-st}f_2(t-t') \\ &= \int_0^\infty \mathrm{d}t'\mathrm{e}^{-st'}f_1(t')\int_{t'}^\infty \mathrm{d}t\mathrm{e}^{-s(t-t')}f_2(t-t') \\ &= \tilde{f}_1(s)\tilde{f}_2(s)\end{aligned} \tag{197}$$

□

Example. Consider the differential equation

$$f'' + 5f' + 6f = 0 \tag{198}$$

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

$$s^2\hat{f}(s) - sf(0) - f'(0) + 5[s\tilde{f}(s) - f(0)] + 6\tilde{f}(s) = \tilde{f}(s)(s^2+5s+6) = \frac{1}{s} \tag{199}$$

rearranging this, we have

$$\tilde{f}(s) = \frac{1}{s(s+2)(s+3)} = \frac{1}{6s} - \frac{1}{2(s+2)} + \frac{1}{3(s+3)} \tag{200}$$

So

$$f(t) = \frac{1}{6} - \frac{1}{2}\mathrm{e}^{-2t} + \frac{1}{3}\mathrm{e}^{-3t} \tag{201}$$

5 Complex Analysis

5.1 Complex Functions of a Complex Variable

A complex number $z = x + iy$ can be mapped to another complex number

$$w = f(z) = u(x, y) + iv(x, y) \tag{202}$$

where $u(x, y)$ and $v(x, y)$ are real functions of the real variables x and y.

It is often useful to use the 'polar representation' of complex numbers where

$$z = r\mathrm{e}^{i\theta} \tag{203}$$

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 Arg(z), which is values $-\pi <$ 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) $f(z) = z^{1/3} = r^{1/3}\mathrm{e}^{(i\theta+2\pi in)/3} = \begin{cases} r^{1/3}\exp\left(\frac{i\theta}{3}\right) \\ r^{1/3}\exp\left(\frac{i\theta}{3} + \frac{2\pi i}{3}\right) \\ r^{1/3}\exp\left(\frac{i\theta}{3} + \frac{4\pi i}{3}\right) \end{cases}$

Complex functions defined as power series

$$\mathrm{e}^z = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \cdots \tag{204}$$

$$\cos z = 1 - \frac{z^2}{2!} + \frac{z^4}{4!} - \cdots \tag{205}$$

$$\ln(1 + z) = z - \frac{z^2}{2} + \frac{z^3}{3} - \cdots \qquad (|z| < 1) \tag{206}$$

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*

$$\lim_{z\to z_0} f(z) = f(z_0) \tag{207}$$

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

$$\lim_{z \to z_0} \frac{f(z) - f(z_0)}{z - z_0} = F \tag{208}$$

we say $f'(z_0) = (\mathrm{d}f/\mathrm{d}z)\big|_{z_0} = F$.

Definition. *A subset $D \in \mathbb{C}$ 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 $z = z_0 + \delta z$

$$\lim_{\delta z \to 0} \frac{(z_0 + \delta z)^2 - z_0^2}{\delta z} = 2z_0 \tag{209}$$

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

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

$$\lim_{\delta z \to 0} \frac{(z_0 + \delta z)^* - z_0^*}{\delta z} = \lim_{\delta z \to 0} \frac{\delta z^*}{\delta z} = \mathrm{e}^{-2i\theta} \tag{210}$$

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

Note. If $f(z)$ has an experience including z only if it will be analytic; If $f(z)$ has an experience including z^*, then it wouldn't be analytic.

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.

$$\frac{\partial f}{\partial x} = \frac{\mathrm{d}f}{\mathrm{d}z}\frac{\partial z}{\partial x} = f', \qquad \frac{\partial f}{\partial y} = \frac{\mathrm{d}f}{\mathrm{d}z}\frac{\partial z}{\partial y} = if' \tag{211}$$

which shows

$$i\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y} \quad \Rightarrow \quad i\left(\frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x}\right) = \left(\frac{\partial u}{\partial y} + i\frac{\partial v}{\partial y}\right) \tag{212}$$

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

$$\boxed{\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \qquad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}} \tag{213}$$

It is a theorem that $f(z)$ is analytic if and only id 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 $v = 2xy$.

$$\frac{\partial u}{\partial x} = 2x, \qquad \frac{\partial u}{\partial y} = -2y \tag{214}$$

$$\frac{\partial v}{\partial x} = 2y, \qquad \frac{\partial v}{\partial y} = 2x \tag{215}$$

satisfy the C-R equations.

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

$$\frac{\partial u}{\partial x} = 1 \neq \frac{\partial v}{\partial y} = 0 \tag{216}$$

C-R equations fail.

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

$$\frac{\partial u}{\partial x} = 2x, \qquad \frac{\partial u}{\partial y} = 2y, \qquad \frac{\partial v}{\partial x} = \frac{\partial v}{\partial y} = 0 \tag{217}$$

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 neighghood of z_0.

$$f(z) = c_0 + c_1(z-z_0) + c_2(z-z_0)^2 + \cdots = \sum_{k=0}^{\infty} c_k(z-z_0)^k \tag{218}$$

where $c_k = f^{(k)}(z_0)/k!$, in a neighbourhood of z_0, for every z_0 in D.

Example. List of analytic functions: $\mathrm{e}^z, \cos z, \sin z, \sinh z, \cosh z, \ln(1+z), \frac{P(z)}{Q(z)}$ where P and Q are polynomials in z (everywhere except at the zeros of Q).

5.2.3 Harmonic Functions

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

Now we look at C-R equations

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial x}\frac{\partial u}{\partial x} = \frac{\partial}{\partial x}\frac{\partial v}{\partial y} = \frac{\partial}{\partial y}\frac{\partial v}{\partial x} = -\frac{\partial}{\partial y}\frac{\partial u}{\partial y} = -\frac{\partial^2 u}{\partial y^2} \tag{219}$$

Hence
$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \nabla^2 u = 0 \tag{220}$$
$u(x, y)$ 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 $u(x, y) = \cos x \cosh y$
$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\cos x \cosh y + \cos x \cosh y = 0 \tag{221}$$
hence u is harmonic. Then we find the conjugate harmonic function $v(x, y)$. Using the C-R equations
$$\frac{\partial v}{\partial y} = \frac{\partial u}{\partial x} = -\sin x \cosh y \quad \Rightarrow \quad v = -\sin x \sinh y + c_1(y) \tag{222}$$
$$\frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y} = -\cos x \sinh y \quad \Rightarrow \quad v = -\sin x \sinh y + c_2(x) \tag{223}$$
so that $c_1 = c_2 = c$ and $v(x, y) = -\sin x \sinh y + c$, where c is a constant. Hence
$$f(z) = \cos x \cosh y - i \sin x \sinh y + \tilde{c} \tag{224}$$
is analytic by construction.

5.3 Multi-Valued Functions

Example. $f(z) = z^{1/3}$. There are three related branches of $z^{1/3}$
$$\begin{cases} F_1(z) = r^{1/3} \mathrm{e}^{i\theta/3} \\ F_2(z) = r^{1/3} \mathrm{e}^{i\theta/3 + 2\pi i/3} \\ F_3(z) = r^{1/3} \mathrm{e}^{i\theta/3 + 4\pi i/3} \end{cases} \tag{225}$$
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
$$f(z) = F_i(z) \quad \text{on sheet } i \tag{226}$$
$f(z)$ is single valued and continuous on the Riemann surface.

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

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

Example. $f(z) = \ln z = \ln\left(r e^{i\theta}\right)$ not defined at $z = 0$.
$$f(z) = \ln r + i\theta + 2\pi i n \tag{227}$$

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 in Fig.4).

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.

5.4 Integration of Complex Functions

5.4.1 Contours

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

Example. Evaluate $\int_c z\mathrm{d}z$ along (i) $y = x^2$ and (ii) $y = x$.

$$\int_C z\mathrm{d}z = \int_C (x + iy)(\mathrm{d}x + i\mathrm{d}y) = \int_C (x\mathrm{d}x - y\mathrm{d}y) + i\int_C (y\mathrm{d}x + x\mathrm{d}y) \tag{228}$$

(i) $\int_0^1 \int (x\mathrm{d}x - 2x^3\mathrm{d}x) + i\int_0^1 (x^2\mathrm{d}x + 2x^2\mathrm{d}x) = i$

(ii) $\int_0^1 (x\mathrm{d}x - x\mathrm{d}x) + i\int_0^1 (x\mathrm{d}x + x\mathrm{d}x) = i$

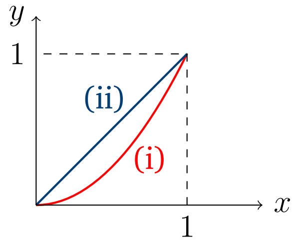

Figure 5: The two paths, (i) $y = x^2$ and (ii) $y = x$, along with the function $f(z)$ is to be integrated in the example.

5.4.2 Cauchy's Theorem

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

$$\oint_C f(z)\mathrm{d}z = 0 \tag{229}$$

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

$$\oint_C (P\mathrm{d}x + Q\mathrm{d}y) = \iint_D \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y}\right) \mathrm{d}x\mathrm{d}y \tag{230}$$

Proof. Use Green's theorem in the plane and Cauchy-Riemann conditions to prove Cauchy's theorem.

$$\begin{aligned}\oint_C f(z)\mathrm{d}z &= \oint_C (u(x,y) + iv(x,y))(\mathrm{d}x + i\mathrm{d}y) \\ &= \oint_C (u\mathrm{d}x - v\mathrm{d}y) + i\oint_C (v\mathrm{d}x + u\mathrm{d}y) \\ &= \iint_D \left(-\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right) \mathrm{d}x\mathrm{d}y + i\iint_D \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right) \mathrm{d}x\mathrm{d}y = 0\end{aligned} \tag{231}$$

□

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

$$\int_{C_1} f(z)\mathrm{d}z = \int_{C_2} f(z)\mathrm{d}z \tag{232}$$

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

$$\oint_C f(z)\mathrm{d}z = \int_{C_1} f(z)\mathrm{d}z - \int_{C_2} f(z)\mathrm{d}z = 0 \tag{233}$$

□

5.4.4 Contour Deformation

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

$$\oint_{C_1} f(z)\mathrm{d}z = \oint_{C_2} f(z)\mathrm{d}z \tag{234}$$

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

$$\begin{aligned}\oint_C f(z)\mathrm{d}z &= \left(\int_{C_1} + \int_{\overline{BA}} - \int_{C_2} + \int_{\overline{AB}}\right) f(z)\mathrm{d}z \\ &= \int_{C_1} f(z)\mathrm{d}z - \int_{C_2} f(z)\mathrm{d}z = 0\end{aligned} \tag{235}$$

□

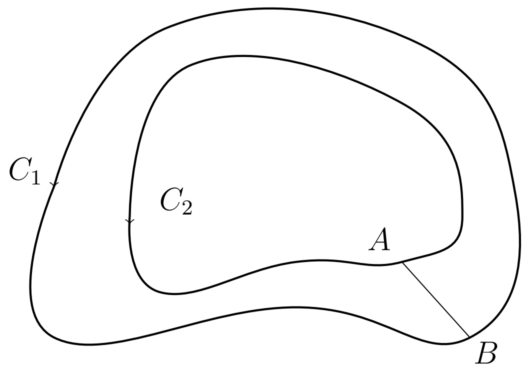

Figure 6: The constructed contour C_1 and C_2 for the proof of contour deformation.

Example. Evaluate $\oint_C \frac{1}{z}\mathrm{d}z$, where C is a closed contour around the original point. Deform the contour into a small circle, radius $r = 1$, centred on the origin

$$z = \mathrm{e}^{i\theta}, \qquad \mathrm{d}z = i\mathrm{e}^{i\theta}\mathrm{d}\theta \tag{236}$$

then

$$\oint_C \frac{1}{z}\mathrm{d}z = \oint_{|z|=1} \frac{1}{z}\mathrm{d}z = \int_{-\pi}^{\pi} \mathrm{e}^{-i\theta} i\mathrm{e}^{i\theta}\mathrm{d}\theta = 2\pi i \tag{237}$$

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

$$\oint_C \frac{f(z)}{z - z_0}\mathrm{d}z = 2\pi i f(z_0) \tag{238}$$

or

$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z - z_0} \mathrm{d}z \tag{239}$$

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.* $C_r : z = z_0 + re^{i\theta}(r \to 0)$, then

$$\begin{aligned} \oint_C \frac{f(z)}{z - z_0} \mathrm{d}z &= \lim_{r\to 0} \oint_{C_r} \frac{f(z)}{z - z_0} \mathrm{d}z = \lim_{r\to 0} \int_0^{2\pi} \frac{f(z_0 + re^{i\theta})}{re^{i\theta}} ire^{i\theta} \mathrm{d}\theta \\ &= \lim_{r\to 0} i \int_0^{2\pi} f(z_0 + re^{i\theta}) \mathrm{d}\theta = 2\pi i f(z_0) \end{aligned} \tag{240}$$

□

Example. Consider the integral

$$\oint \frac{\sin z}{z^2 + 1} \mathrm{d}z = \oint_C \frac{\sin z}{(z + i)(z - i)} \mathrm{d}z \tag{241}$$

and consider the closed contour (1) C and (2) $\tilde{C}$.

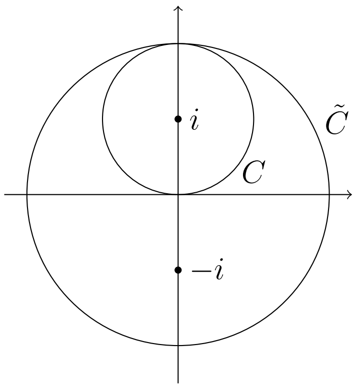

Figure 7: The contour C and $\tilde{C}$ for the example.

(1) For the contour C, We choose

$$f(z) = \frac{\sin z}{z + i} \tag{242}$$

Then

$$\oint_C \frac{\sin z}{z^2 + 1} \mathrm{d}z = \oint_C \frac{f(z)}{z - i} \mathrm{d}z = 2\pi i \frac{\sin i}{2i} = \pi i \sinh 1 \tag{243}$$

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

$$\begin{aligned} \oint_{\tilde{C}} \frac{\sin z}{z^2 + 1} \mathrm{d}z &= \oint_{\tilde{C}} \frac{\sin z}{(z + i)(z - i)} \mathrm{d}z = \frac{i}{2} \oint_{\tilde{C}} \left(\frac{\sin z}{z + i} - \frac{\sin z}{z - i} \right) \mathrm{d}z \\ &= -\pi(\sin(-i) - \sin(i)) = 2\pi i \sinh 1 \end{aligned} \tag{244}$$

5.4.6 Derivatives of Analytic Functions

Cauchy's integral theorem gives

$$f(z_0) = \frac{1}{2\pi i}\oint_C \frac{f(z)}{z - z_0}\mathrm{d}z \tag{245}$$

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

$$f'(z_0) = \frac{1}{2\pi i}\oint_C \frac{f(z)}{(z - z_0)^2}\mathrm{d}z \tag{246}$$

Similarly,

$$f''(z_0) = \frac{2!}{2\pi i}\oint_C \frac{f(z)}{(z - z_0)^3}\mathrm{d}z \tag{247}$$

$$\vdots$$

$$f^{(n)}(z_0) = \frac{n!}{2\pi i}\oint_C \frac{f(z_0)}{(z - z_0)^{n+1}}\mathrm{d}z \tag{248}$$

Example. Consider the integral

$$I = \oint_C \frac{1}{z^n}\mathrm{d}z = \oint_C \frac{f(z)}{z^{n+1}}\mathrm{d}z \quad \text{with} \quad C : |z| = r \tag{249}$$

with $f(z) = z$, $f'(z) = 1$ and $f^{(n)}(z) = 0 (n \geq 2)$.

- $n = 1$, $I = 2\pi i f(0) = 2\pi i$
- $n \geq 2$, $I = \frac{2\pi i}{n!} f^{(n)}(0) = 0$

5.4.7 Fourier Transform of a Gaussian

We have known that

$$\int_{-\infty}^{\infty} \mathrm{e}^{-x^2}\mathrm{d}x = \int_{-\infty}^{\infty} \mathrm{e}^{-(x'+ia)^2}\mathrm{d}x' \tag{250}$$

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

$$I_1 = \int_{-\infty}^{\infty} \mathrm{e}^{-x^2}\mathrm{d}x = \int_{C_1} \mathrm{e}^{-z^2}\mathrm{d}z \tag{251}$$

$$I_2 = \int_{-\infty}^{\infty} \mathrm{e}^{-(x'+ia)^2}\mathrm{d}x' = \int_{C_2} \mathrm{e}^{-z^2}\mathrm{d}z \tag{252}$$

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 $C_R = C_{1R} + E_R^+ - C_{2R} + E_R^-$. And we have

$$\oint_{C_R} \mathrm{e}^{-z^2}\mathrm{d}z = 0 \tag{253}$$

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

$$\lim_{R\to\infty} \oint_{C_R} \mathrm{e}^{-z^2} \mathrm{d}z = \lim_{R\to\infty} \left(\int_{C_1} + \int_{E_R^+} - \int_{C_2} + \int_{E_R^-} \right) \mathrm{e}^{-z^2} \mathrm{d}z = 0 \tag{254}$$

Now

$$\lim_{R\to\infty} \int_{E_R^+} \mathrm{e}^{-z^2} \mathrm{d}z = \lim_{R\to\infty} \int_0^a \mathrm{e}^{-(R+iy)^2} i\mathrm{d}y = 0 \tag{255}$$

$$\lim_{R\to\infty} \int_{E_R^-} \mathrm{e}^{-z^2} \mathrm{d}z = \lim_{R\to\infty} \int_a^0 \mathrm{e}^{-(-R+iy)^2} i\mathrm{d}y = 0 \tag{256}$$

So we have $I_1 = I_2$. □

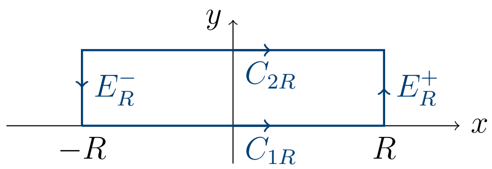

Figure 8: The contour C_R.

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

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_n)^2 \tag{257}$$

where

$$a_n = \frac{f^{(n)}(z_0)}{n!} = \frac{1}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^{n+1}} \mathrm{d}z \tag{258}$$

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.

$$f(z) = \frac{\mathrm{e}^z}{(z-5)(z+i)(z-(1+i))^2} \tag{259}$$

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.*
$$f(z) = \frac{g(z)}{(z-z_0)^m} \tag{260}$$
This implies $f(z)$ has a power series except around z_0
$$f(z) = \sum_{n=0}^{\infty} a_n (z-z_0)^n + \sum_{n=1}^{m} \frac{b_n}{(z-z_0)^n} \tag{261}$$
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
$$f(z) = \sum_{n=0}^{\infty} a_n (z-z_0)^n + \sum_{n=1}^{\infty} \frac{b_n}{(z-z_0)^n} \tag{262}$$

Example.
$$f(z) = \mathrm{e}^{1/z} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{1}{z}\right)^n \tag{263}$$

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*
$$\mathrm{Res}_f(z_0) = \frac{1}{2\pi i} \oint_{C_{z_0}} f(z) \mathrm{d}z \tag{264}$$
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
$$f(z) = \frac{g(z)}{(z-z_0)^m} \tag{265}$$
and
$$\mathrm{Res}_f(z_0) = \frac{1}{2\pi i} \oint_C \frac{g(z)}{(z-z_0)^m} \mathrm{d}z = \frac{1}{(m-1)!} \frac{\mathrm{d}^{m-1} g(z)}{\mathrm{d}z^{m-1}} \bigg|_{z=z_0} \tag{266}$$

Example.

(1) $f(z) = 1/(z-z_0)$
$$\mathrm{Res}_f(z_0) = 1 \tag{267}$$

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

$$\mathrm{Res}_f(-1) = \left.\frac{\mathrm{d}\sin z}{\mathrm{d}z}\right|_{z=-1} = \cos(-1) = \cos 1 \tag{268}$$

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

$$\oint_C f(z)\mathrm{d}z = 2\pi i \sum_{k=1}^{N} \mathrm{Res}_f(z_k) \tag{269}$$

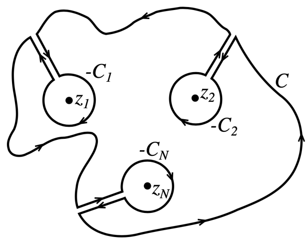

Figure 9: The contour C used in the proof of the residue theorem.

Proof. Construct the closed contour $\tilde{C} = C-(C_1+C_2+C_3)$. $f(z)$ is analytic anywhere inside $\tilde{C}$. By Cauchy's theorem

$$\oint_{\tilde{C}} f(z)\mathrm{d}z = \oint_C f(z)\mathrm{d}z - 2\pi i \sum_{k=1}^{N} \mathrm{Res}_f(z_k) = 0 \tag{270}$$

□

5.6.2 Contour Integration Examples

Example.

(1)

$$I = \oint_{|z|=1} \mathrm{e}^{1/z}\mathrm{d}z = \oint_{|z|=1} \left[1 + \frac{1}{z} + \frac{1}{2!}\left(\frac{1}{z}\right)^2 + \cdots\right]\mathrm{d}z = 2\pi i \tag{271}$$

(2)

$$\begin{aligned} I = &\oint_{|z|=3} \frac{z+2}{2z^2+1}\mathrm{d}z = \oint_{|z|=3} \frac{z+2}{2(z+\frac{i}{\sqrt{2}})(z-\frac{i}{\sqrt{2}})}\mathrm{d}z \\ =&2\pi i\left[\mathrm{Res}\left(\frac{i}{\sqrt{2}}\right) + \mathrm{Res}\left(-\frac{i}{\sqrt{2}}\right)\right] \\ =&2\pi i\left[\frac{\frac{i}{\sqrt{2}}+2}{2(\frac{i}{\sqrt{2}}+\frac{i}{\sqrt{2}})} + \frac{-\frac{i}{\sqrt{2}}+2}{2(-\frac{i}{\sqrt{2}}-\frac{i}{\sqrt{2}})}\right] = \pi i \end{aligned} \tag{272}$$

(3)

$$I=\int_{-\infty}^{\infty}\frac{\mathrm{d}x}{(x^2+1)(x^2+9)} \tag{273}$$

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

$$\begin{aligned}
I=&\lim_{R\to\infty}\int_{-R}^{R}\frac{\mathrm{d}x}{(x^2+1)(x^2+9)}=\lim_{R\to\infty}\int_{S_R}\frac{\mathrm{d}z}{(z^2+1)(z^2+9)}\\
=&\lim_{R\to\infty}\oint_{C}\frac{\mathrm{d}z}{(z+i)(z-i)(z+3i)(z-3i)}-\lim_{R\to\infty}\int_{C_R}\frac{\mathrm{d}z}{(z^2+1)(z^2+9)}\\
=&2\pi i\left[\mathrm{Res}(i)+\mathrm{Res}(3i)\right]-\lim_{R\to\infty}\frac{iR}{(R^2+1)(R^2+9)}\int_0^{\pi}\mathrm{e}^{i\theta}\mathrm{d}\theta\\
=&2\pi i\left(\frac{1}{16i}+\frac{1}{-48i}\right)=\frac{\pi}{12}
\end{aligned} \tag{274}$$

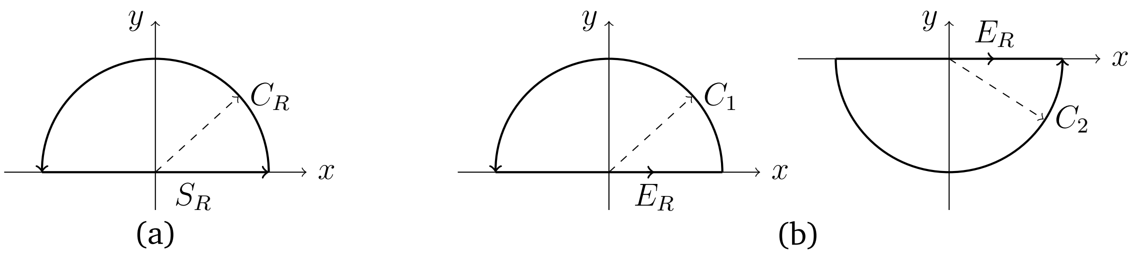

Figure 10: (a) The contour for example (3). (b) The contour for example (4).

(4)

$$\begin{aligned}
I=&\int_{-\infty}^{\infty}\frac{\cos x}{x^2+1}\mathrm{d}x=\int_{x-\text{axis}}\frac{\cos z}{z^2+1}\mathrm{d}z\\
=&\int_{x-\text{axis}}\frac{\mathrm{e}^{iz}}{2(z+i)(z-i)}\mathrm{d}z+\int_{x-\text{axis}}\frac{\mathrm{e}^{-iz}}{2(z+i)(z-i)}\mathrm{d}z\\
=&I_1+I_2
\end{aligned} \tag{275}$$

Consider the closed contour $\tilde{C}_1=C_1+E_R$ and $\tilde{C}_2=C_2-E_R$ (see in fig.10(b))

$$\begin{aligned}
I_1=&\lim_{R\to\infty}\oint_{\tilde{C}_1}\frac{\mathrm{e}^{iz}}{2(z+i)(z-i)}\mathrm{d}z-\lim_{R\to\infty}\int_{C_1}\frac{\mathrm{e}^{iz}}{2(z+i)(z-i)}\mathrm{d}z\\
=&2\pi i\,\mathrm{Res}(i)-\lim_{R\to\infty}\int_0^{\pi}\frac{\mathrm{e}^{iR\mathrm{e}^{i\theta}}}{2(R^2+1)}iR\mathrm{e}^{i\theta}\mathrm{d}\theta=2\pi i\frac{\mathrm{e}^{-1}}{4i}-0=\frac{\pi}{2}\mathrm{e}^{-1}
\end{aligned} \tag{276}$$

$$\begin{aligned}
I_2=&-\lim_{R\to\infty}\oint_{\tilde{C}_2}\frac{\mathrm{e}^{-iz}}{2(z+i)(z-i)}\mathrm{d}z+\lim_{R\to\infty}\int_{C_2}\frac{\mathrm{e}^{-iz}}{2(z^2+1)}\mathrm{d}z\\
=&-2\pi i\,\mathrm{Res}(-i)+\lim_{R\to\infty}\int_{-\pi}^{0}\frac{\mathrm{e}^{-iR\mathrm{e}^{i\theta}}}{2(R^2+1)}iR\mathrm{e}^{i\theta}\mathrm{d}\theta\\
=&-2\pi i\frac{\mathrm{e}^{-1}}{-4i}+0=\frac{\pi}{2}\mathrm{e}^{-1}
\end{aligned} \tag{277}$$

So we have

$$I = I_1 + I_2 = \pi e^{-1} \tag{278}$$

5.6.3 Inverting Laplace Transforms

Suppose we know

$$F(s) = \mathcal{L}[f(t)] = \int_0^s f(t)e^{-st}dt \tag{279}$$

and we want to find

$$f(t) = \mathcal{L}^{-1}[F(s)] = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} F(s)e^{st}ds \tag{280}$$

which is called *Bromwich integral*.To invert a Laplace transform $F(s)$. There are steps to help find the solution

(1) Find the singular points $a_1, a_2, \cdots$ of $F(s)$ and choose a real number c such that $c > \mathrm{Re}(a_i)$ for all i.

(2) Close the Bromwich integral contour show in Fig.11 with a large semicircle in the left-hand half-plane.

(3) If the integral around the semicircle vanished as $R \to \infty$, then

$$f(t) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} F(s)e^{st}ds = \sum_i \mathrm{Res}(a_i) - \lim_{R\to\infty}\int_{C_R} F(s)e^{st}ds \tag{281}$$

where $\mathrm{Res}(a_i)$ is the residues of $F(s)e^{st}$. Here we notice $e^{st} = e^{xt+iyt}$. As we close the contour to the left, *i.e.*, $x \to -\infty$. So $e^{st} \to 0(t>0)$. Hence

$$f(t) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} F(s)e^{st}ds = \sum_i \mathrm{Res}(a_i), \qquad t > 0 \tag{282}$$

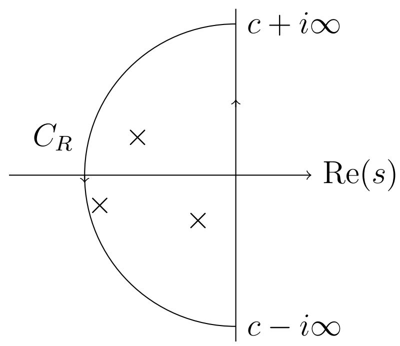

Figure 11: The contour for inverting Laplace transforms.

6 Calculus of Variations

6.1 Introduction

A **function** f maps a number, x, to another number, $f(x)$

$$x \;\rightarrow\; \boxed{f} \;\rightarrow\; f(x)$$

A **functional** I maps a function, f, to a number $I[f]$

$$y(x) \;\rightarrow\; \boxed{I} \;\rightarrow\; I[y(x)]$$

Example.

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

(2) $T(\psi) = \int \psi^*(x)\frac{\hat{p}^2}{2m}\psi(x)\mathrm{d}x$

(3) $U(\rho) = \frac{1}{2}\iint \frac{\rho(\boldsymbol{r})\rho(\boldsymbol{r}')}{4\pi\varepsilon_0|\boldsymbol{r}-\boldsymbol{r}'|}\mathrm{d}^3\boldsymbol{r}\mathrm{d}^3\boldsymbol{r}'$

(4) $S[y] = \int_a^b \sqrt{1+(\frac{\mathrm{d}y}{\mathrm{d}x})^2}\mathrm{d}x =$ length of curve from $x=a$ to $x=b$ given by $y(x)$.

(5) $S[x] = \int_{t_1}^{t_2}\left[\frac{1}{2}m\dot{x}^2 - V(x)\right]\mathrm{d}t =$ action.

Calculus is to find stationary points x_0 of $f(x)$

$$f(x+\delta x) = f(x) + \delta x f'(x) + \frac{(\delta x)^2}{2}f''(x) + \cdots \tag{283}$$

At a stationary point $x = x_0$

$$f'(x_0) = 0 \tag{284}$$

$$\delta f(x) = f(x+\delta x) - f(x) = \mathcal{O}(\delta x^2) \tag{285}$$

Calculus of variations is to find a stationary function of the functional $I[y]$

$$\delta I = I[y+\delta y] - I[y] \tag{286}$$

Seek $y = y_0$ such that

$$\delta I|_{y_0} = \mathcal{O}(\delta y^2) \tag{287}$$

6.2 The Euler-Lagrange Problem

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

$$I[y] = \int_{x_A}^{x_B} f(x, y(x), y'(x))\mathrm{d}x \tag{288}$$

where f is a function of 3 arguments x, y, y', 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 y is a stationary function of I or I is stationary at y.

Consider varying $y(x)$ slightly

$$y(x) \to y(x) + \delta y(x) \tag{289}$$

then

$$\begin{aligned} I[y+\delta y] &= \int_{x_A}^{x_B} f(x, y(x) + \delta y(x), y' + \delta y'(x)) \mathrm{d}x \\ &= \int_{x_A}^{x_B} \left[f(x,y,y') + \delta y \frac{\partial f}{\partial y} + \delta y' \frac{\partial f}{\partial y'} + \mathcal{O}(\delta y^2) \right] \mathrm{d}x \end{aligned} \tag{290}$$

so we have

$$\begin{aligned} \delta I =& I[y+\delta y] - I[y] \\ =& \int_{x_A}^{x_B} \left(\delta y \frac{\partial f}{\partial y} + \delta y' \frac{\partial f}{\partial y'} \right) \mathrm{d}x + \mathcal{O}(\delta y^2) \\ =& \int_{x_A}^{x_B} \left(\delta y \frac{\partial f}{\partial y} \right) \mathrm{d}x + \left[\delta y \frac{\partial f}{\partial y'} \right]_{x_A}^{x_B} - \int_{x_A}^{x_B} \delta y \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\partial f}{\partial y'} \right) \mathrm{d}x + \mathcal{O}(\delta y^2) \\ =& \int_{x_A}^{x_B} \delta y \left[\frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\partial f}{\partial y'} \right) \right] \mathrm{d}x + \mathcal{O}(\delta y^2) \end{aligned} \tag{291}$$

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

$$\boxed{\frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\partial f}{\partial y'} \right) = 0} \tag{292}$$

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

Example.

$$f(x,y,y') = (1+x^2)y'^2 - y^4 \tag{293}$$

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

$$-4y^3 - \frac{\mathrm{d}}{\mathrm{d}x} \left[(1+x^2)2y' \right] = 0 \tag{294}$$

We can also use the original method of calculus of variations

$$I[y+\delta y] = \int_{x_A}^{x_B} \left[(1+x^2)(y'+\delta y')^2 - (y+\delta y)^4 \right] \mathrm{d}x \tag{295}$$

so

$$\begin{aligned} \delta I =& \int_{x_A}^{x_B} \left[(1+x^2)2y'\delta y' - 4y^3 \delta y \right] \mathrm{d}x \\ =& (1+x^2)2y'\delta y \Big|_{x_A}^{x_B} - \int_{x_A}^{x_B} \mathrm{d}x \left(\delta y \frac{\mathrm{d}}{\mathrm{d}x} [(1+x^2)2y'] + 4y^3 \delta y \right) \mathrm{d}x \\ =& \int_{x_A}^{x_B} \mathrm{d}x \delta y \left(-\frac{\mathrm{d}}{\mathrm{d}x} [(1+x^2)2y'] - 4y^3 \right) \mathrm{d}x \end{aligned} \tag{296}$$

I is stationary if

$$-\frac{\mathrm{d}}{\mathrm{d}x}[(1+x^2)2y'] - 4y^3 = 0 \tag{297}$$

6.2.1 Beltrami identity

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

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}x} + \frac{\partial f}{\partial y'}\frac{\mathrm{d}y'}{\mathrm{d}x} \tag{298}$$

If y is a solution function of the Euler-Lagrange equation

$$\begin{aligned}\frac{\mathrm{d}f}{\mathrm{d}x} =& \frac{\partial f}{\partial x} + y'\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'}\right) + y''\frac{\partial f}{\partial y'} \\ =& \frac{\partial f}{\partial x} + \frac{\mathrm{d}}{\mathrm{d}x}\left(y'\frac{\partial f}{\partial y'}\right)\end{aligned} \tag{299}$$

Suppose f has no explicit dependence on x, *i.e.*, $\partial f/\partial x = 0$, then

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(f - \frac{\partial f}{\partial y'}y'\right) = 0 \tag{300}$$

which integrates to

$$\boxed{f - \frac{\partial f}{\partial y'}y' = \text{const}} \tag{301}$$

This equation is called *Beltrami identity*, which is the first integral of Euler-Lagrange equation.

Example.

$$I[y] = \int f\mathrm{d}x \quad \text{with} \quad f(y, y') = y'^2 - y^4 \tag{302}$$

Applying the Beltrami identity

$$y'^2 - y^4 - 2y'^2 = \text{const} \tag{303}$$

6.2.2 Functional Derivatives

We know that

$$\delta I = \int_{x_A}^{x_B} \delta y \left[\frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'}\right)\right] \mathrm{d}x + \mathcal{O}(\delta y^2) \tag{304}$$

then we can define the *functional derivative of* I with respect to y

$$\frac{\delta I}{\delta y(x)} = \frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'}\right) \tag{305}$$

then Euler-Lagrange equation can be written as[2]

$$\frac{\delta I}{\delta y(x)} = 0 \tag{306}$$

[2]Confer function derivative $\mathrm{d}y/\mathrm{d}x = 0$.

6.2.3 Lagrangian Mechanics

The Lagrangian of a classical particle moving in three dimensions is

$$L = T - V = \frac{1}{2}m\dot{\boldsymbol{x}}^2 + V(\boldsymbol{x}, t) \tag{307}$$

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

$$S[\boldsymbol{x}(t)] = \int_{t_A}^{t_B} L(t, \boldsymbol{x}, \dot{\boldsymbol{x}})\mathrm{d}t \tag{308}$$

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

$$\frac{\partial L}{\partial x_i} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}_i}\right) = 0, \qquad i = 1, 2, 3 \tag{309}$$

these give

$$m\ddot{x}_i = -\nabla_i V, \qquad i = 1, 2, 3 \tag{310}$$

which is Newton's equation.

6.2.4 Examples

Example.

(1) **Shortest Path Problem**
(Method 1)
Between (x, y) and $(x + \mathrm{d}x, y + \mathrm{d}y)$ along curve $y(x)$, the distance is

$$\mathrm{d}s = \sqrt{\mathrm{d}x^2 + \mathrm{d}y^2} = \sqrt{1 + \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2}\mathrm{d}x \tag{311}$$

so the length of $y(x)$ is

$$\int \mathrm{d}s = \int_{x_A}^{x_B} \sqrt{1 + y'^2}\mathrm{d}x \tag{312}$$

This extremised by Euler-Lagrange equation

$$0 - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{y'}{\sqrt{1 + y'^2}}\right) = 0 \quad \Rightarrow \quad y' = c \quad \Rightarrow \quad y = cx + d \tag{313}$$

(Method 2)
We write the curve in *parametrised* form

$$y = y(\lambda), \qquad x = x(\lambda) \tag{314}$$

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

$$\int \mathrm{d}s = \int \sqrt{\mathrm{d}x^2 + \mathrm{d}y^2} = \int_{\lambda_A}^{\lambda_B} \sqrt{\left(\frac{\mathrm{d}x}{\mathrm{d}\lambda}\right)^2 + \left(\frac{\mathrm{d}y}{\mathrm{d}\lambda}\right)^2}\mathrm{d}\lambda \tag{315}$$

This extremised by Euler-Lagrange equation. For x

$$0 - \frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\frac{x'}{\sqrt{x'^2+y'^2}}\right) = 0 \quad \Rightarrow \quad \frac{x'}{\sqrt{x'^2+y'^2}} = \alpha \tag{316}$$

Similarly, for y

$$0 - \frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\frac{y'}{\sqrt{x'^2+y'^2}}\right) = 0 \quad \Rightarrow \quad \frac{y'}{\sqrt{x'^2+y'^2}} = \beta \tag{317}$$

So we have

$$\frac{y'}{x'} = \gamma \quad \Rightarrow \quad \frac{\mathrm{d}y}{\mathrm{d}x} = \gamma \quad \Rightarrow \quad y = \gamma x + c \tag{318}$$

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

$$T = \int_A^B \mathrm{d}t = \int_A^B \frac{\mathrm{d}s}{v} = \int_{x=0}^{x=x_B} \frac{\sqrt{1+y'^2}}{\sqrt{2gy}}\mathrm{d}x \tag{319}$$

Using the Beltrami identity

$$\frac{\sqrt{1+y'^2}}{\sqrt{2gy}} - \frac{\frac{y'}{\sqrt{1+y'^2}}}{\sqrt{2gy}}y' = c \quad \Rightarrow \quad y(1+y'^2) = c^2 \quad \Rightarrow \quad y' = \sqrt{\frac{\alpha - y}{y}} \tag{320}$$

where $\alpha = c^2$. The solution is a cycloid[3]

$$x = x(\theta) = a(\theta - \sin\theta) \tag{321}$$

$$y = y(\theta) = a(1 - \cos\theta) \tag{322}$$

where $a = \alpha/2$. Then we can find the total time along the cycloid from A to B in terms of θ_B

$$T = \int_0^{\theta_B} \frac{\sqrt{(\mathrm{d}x/\mathrm{d}\theta)^2 + (\mathrm{d}y/\mathrm{d}\theta)^2}}{\sqrt{2gy}}\mathrm{d}\theta = \int_0^{\theta_B}\sqrt{\frac{a}{g}}\mathrm{d}\theta = \sqrt{\frac{a}{g}}\theta_B \tag{323}$$

6.2.5 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

$$L(x, \dot{x}) = T - L = \frac{1}{2}m\dot{x}^2 - V(x) \tag{324}$$

[3]Hint: suppose $\tan\phi = \sqrt{\frac{y}{\alpha - y}}(-\pi/2 < \phi < \pi/2)$.

Using the Beltrami identity

$$L - \frac{\partial L}{\partial \dot{x}}\dot{x} = \text{const} \tag{325}$$

which gives

$$\frac{1}{2}m\dot{x}^2 + V = \underbrace{T + V}_{\text{total energy}} = \text{const} \tag{326}$$

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 $\boldsymbol{q}$

$$L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = T - V(\boldsymbol{q}), \qquad \boldsymbol{q} = (q_1, q_2, \cdots, q_N) \tag{327}$$

which does not depend on t. If one defines

$$H = -L + \sum_{i=1}^{N} \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} \tag{328}$$

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 $V(\boldsymbol{x}, \dot{\boldsymbol{x}}, t)$ is independent of $\boldsymbol{x} = (x_1, x_2, x_3)$, *i.e.*, there is no extended force in x_i direction

  $$\frac{\partial V}{\partial x_i} = 0, \qquad i = 1, 2, 3 \tag{329}$$

  The Lagrangian is also independent of $\boldsymbol{x}$. The Euler-Lagrange equation gives

  $$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}_i}\right) = 0 \quad \Rightarrow \quad m\dot{x}_i = \text{const} \tag{330}$$

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

- **Conservation of angular momentum**
  Suppose $\boldsymbol{q} = (r(t), \theta(t).\phi(t))$, then the Lagrangian for the particle is

  $$L = T - V(r, \theta, \phi) \tag{331}$$

  where the kinetic energy

  $$T = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2 + r^2 \sin^2\theta\dot{\phi}^2) \tag{332}$$

  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.

  $$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{\phi}}\right) = \frac{\partial L}{\partial \phi} = 0 \quad \Rightarrow \quad mr^2\sin^2\theta\dot{\phi} = \text{const} \tag{333}$$

  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.

6.3 Constrain Extremisation and Lagrange Multipliers

6.3.1 Constrained Extremisation of Functions

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

$$g(x, y) - C = 0 \tag{334}$$

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

$$\boldsymbol{\nabla} f(P) \parallel \boldsymbol{\nabla} g(P) \quad \Rightarrow \quad \boldsymbol{\nabla}\left(f(x, y) - \lambda g(x, y)\right)_P = 0 \tag{335}$$

The gradient ratio $\lambda(\neq 0)$, is called a *Lagrange multiplier*.

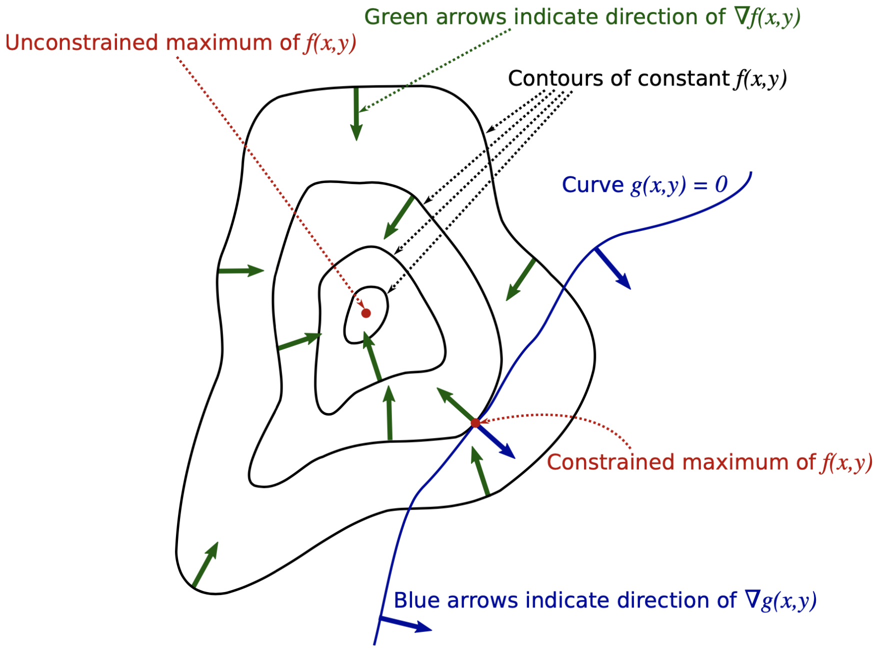

Figure 12: An illustration of the method of Lagrange multipliers.

In d-dimension, with the function $f(x_1, \cdots, x_d)$ and more constraints

$$\begin{aligned} g_1(\boldsymbol{x}) &= C_1 \\ g_2(\boldsymbol{x}) &= C_2 \\ &\vdots \\ g_k(\boldsymbol{x}) &= C_k \end{aligned} \tag{336}$$

The constraint surface is $d-k$ dimensional. f is extremised on the constraint surface if

$$\boldsymbol{\nabla}(f - \lambda_1 g_1 - \lambda_2 g_2 - \cdots - \lambda_k g_k) = 0 \tag{337}$$

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

$$f(x_1, x_2, y_1, y_2) = (x_2 - x_1)^2 + (y_2 - y_1)^2 \tag{338}$$

Construct

$$u(x_1, x_2, y_1, y_2) = f(x_1, x_2, y_1, y_2) + \lambda_1 x_1 y_1 + \mu(x_2 + 2y_2) \tag{339}$$

$\nabla u = 0$ gives

$$\frac{\partial u}{\partial x_1} = 2(x_1 - x_2) + \lambda_1 y_1 = 0 \tag{340}$$

$$\frac{\partial u}{\partial x_2} = 2(x_2 - x_1) + \mu_2 = 0 \tag{341}$$

$$\frac{\partial u}{\partial y_1} = 2(y_1 - y_2) + \lambda_1 x_1 = 0 \tag{342}$$

$$\frac{\partial u}{\partial y_2} = 2(y_2 - y_1) + 2\mu_2 = 0 \tag{343}$$

The solution is

$$(x_1, y_1) = \left(\sqrt{2}, \frac{\sqrt{2}}{2}\right), \qquad (x_2, y_2) = \left(\frac{1 + 3\sqrt{2}}{5}, \frac{4 - 3\sqrt{2}}{10}\right) \tag{344}$$

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

6.3.2 Constrained Extremisation 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 $\mathrm{d}m = \rho \mathrm{d}s$. The total energy

$$E = g\int_A^B y\mathrm{d}m = \rho g \int_A^B y\mathrm{d}s = \rho g \int_{-a}^{a} y\sqrt{1 + \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2}\mathrm{d}x \tag{345}$$

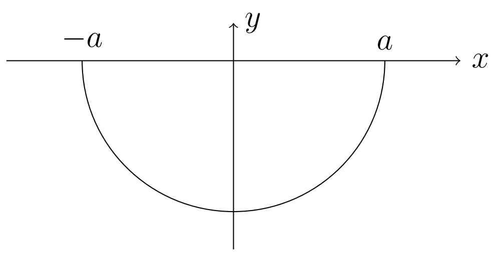

Figure 13: A heavy rope of a chain hanging between two fixed end points $A(-a, 0)$ and $B(a, 0)$.

The length of the rope is fixed. So the constraint

$$L = \int_A^B \mathrm{d}s = \int_{-a}^{a} \sqrt{1 + \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2} \mathrm{d}x \tag{346}$$

Then we have to extremise

$$\begin{aligned} U = E - \lambda L =& \rho g \int_{-a}^{a} y \sqrt{1 + \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2} \mathrm{d}x - \lambda \int_{-a}^{a} \sqrt{1 + \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2} \mathrm{d}x \\ =& \int_{-a}^{a} (\rho g y - \lambda) \sqrt{1 + y'^2} \mathrm{d}x = \int_{-a}^{a} f \mathrm{d}x \end{aligned} \tag{347}$$

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

$$f - \frac{\partial f}{\partial y'} y' = C \tag{348}$$

which is

$$(\rho g y - \lambda)\sqrt{1 + y'^2} - (\rho g y - \lambda)\frac{y'^2}{\sqrt{1 + y'^2}} = C \tag{349}$$

$$\rho g y - \lambda = C\sqrt{1 + y'^2} \tag{350}$$

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

$$\eta = C\sqrt{1 + \frac{\eta'^2}{\rho^2 g^2}}, \qquad \eta' = \pm \rho g \sqrt{\frac{\eta^2}{C^2} - 1} \tag{351}$$

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

$$\eta' = \frac{\mathrm{d}\eta}{\mathrm{d}x} = \rho g \sqrt{\frac{\eta^2}{C^2} - 1} \quad \Rightarrow \quad \frac{\mathrm{d}\eta}{\sqrt{\frac{\eta^2}{C^2} - 1}} = \rho g \mathrm{d}x \tag{352}$$

Let $\eta = C\cosh q$, then $\mathrm{d}\eta = C\sinh q \mathrm{d}q$

$$\begin{aligned} &\int \frac{\mathrm{d}\eta}{\sqrt{\frac{\eta^2}{C^2} - 1}} = \rho g \int \mathrm{d}x \\ \Rightarrow \quad & C \int \mathrm{d}q = \rho g \mathrm{d}x \\ \Rightarrow \quad & Cq = \rho g x + d \\ \Rightarrow \quad & \frac{\eta}{C} = \cosh\left(\frac{\rho g x + d}{C}\right) \end{aligned} \tag{353}$$

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

$$y(x) = \frac{1}{\rho g}\left[\cosh\left(\frac{\rho g x}{C}\right) + \lambda\right] \tag{354}$$

The two constraints

1. When $x = a$, $y = 0$
$$\frac{1}{\rho g}\left[\cosh\left(\frac{\rho g a}{C} + \lambda\right)\right] = 0 \tag{355}$$

2. The length of the rope is fixed
$$L = \int_{-a}^{a} \cosh\left(\frac{\rho g x}{C}\right) \mathrm{d}x = \frac{C}{\rho g} \sinh \frac{\rho g x}{C}\bigg|_{-a}^{a} = \frac{2C}{\rho g} \sinh \frac{\rho g a}{C} \tag{356}$$

Then we can find numerically solutions for C and λ from the constraints above.

6.4 Variational Methods for Solving the Schrödinger Equation

6.4.1 Variational Formulation of 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

$$E[\psi] = \int \psi^* \hat{H} \psi \tag{357}$$

subject to the normalisation constraint

$$\int \psi^* \psi = 1 \tag{358}$$

We claim that
$$I[\psi] = \int \psi^* \hat{H} \psi - \varepsilon \int \psi^* \psi \tag{359}$$

Here ε is the eigenvalue. Let ψ extremes I, we have

$$\begin{aligned}
\delta I =& I[\psi + \delta\psi] - I[\psi] \\
=& \int (\delta\psi^*) \hat{H} \psi + \int \psi^* \hat{H}(\delta\psi) - \varepsilon \int (\delta\psi^*)\psi - \varepsilon \int \psi^*(\delta\psi) \\
=& \int (\delta\psi^*)(\hat{H}\psi - \varepsilon\psi) + \int (\delta\psi)(\hat{H}\psi - \varepsilon\psi)^* = 0
\end{aligned} \tag{360}$$

$$\begin{aligned}
\delta I =& I[\psi + i\delta\psi] - I[\psi] \\
=& -i \int (\delta\psi^*) \hat{H} \psi + i \int \psi^* \hat{H}(\delta\psi) + i\varepsilon \int (\delta\psi^*)\psi - i\varepsilon \int \psi^*(\delta\psi) \\
=& -i \int (\delta\psi^*)(\hat{H}\psi - \varepsilon\psi) + i \int (\delta\psi)(\hat{H}\psi - \varepsilon\psi)^* = 0
\end{aligned} \tag{361}$$

Compare the two equations, we have

$$\int (\delta\psi^*)(\hat{H}\psi - \varepsilon\psi) = 0 \tag{362}$$

for any ψ. Hence
$$\hat{H}\psi - \varepsilon\psi = 0 \tag{363}$$

6.4.2 The Linear Variational Method

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

$$\tilde{\psi}(\boldsymbol{c}) = \sum_{\alpha=1}^{M} c_\alpha \phi_\alpha \tag{364}$$

where $\boldsymbol{c} = (c_1, \cdots, c_M)$ is an M-dimensional vector of expansion coefficients to be determine. Our task is to extremise

$$I[\tilde{\psi}] = I[\boldsymbol{c}] = E[\boldsymbol{c}] - \varepsilon N[\boldsymbol{c}] \tag{365}$$

Here, E is the total energy of the system

$$E[\boldsymbol{c}] = \int \sum_{\alpha=1}^{M} c_\alpha^* \phi_\alpha^* \hat{H} \sum_{\beta=1}^{M} c_\beta \phi_\beta = \sum_{\alpha,\beta=1}^{M} c_\alpha^* H_{\alpha\beta} c_\beta \tag{366}$$

and N is the normalisation constraint.

$$N[\boldsymbol{c}] = \int \sum_{\alpha}^{M} c_\alpha^* \phi_\alpha^* \sum_{\beta}^{M} c_\beta \phi_\beta = \int \sum_{\alpha,\beta=1}^{M} c_\alpha^* S_{\alpha\beta} c_\beta \tag{367}$$

where

$$H_{\alpha\beta} = \int \phi_\alpha^* \hat{H} \phi_\beta = \text{Hamiltonian matrix} \tag{368}$$

$$S_{\alpha\beta} = \int \phi_\alpha^* \phi_\beta = \text{overlap matrix} \tag{369}$$

$S_{\alpha\beta} = \delta_{\alpha\beta}$ 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.