Imperial College London

NOTES

IMPERIAL COLLEGE LONDON

DEPARTMENT OF PHYSICS

Mathematical Methods for Physicists

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Happy New Year :D

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1 Vector Spaces and Tensors

1.1 vector spaces

1.1.1 Definition of a Vector Space

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

1. *$\mathbb{V}$ is closed under **addition**: $\forall \boldsymbol{u}, \boldsymbol{v} \in \mathbb{V} \Rightarrow \boldsymbol{u} + \boldsymbol{v} \in \mathbb{V}$.*
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. $\langle \boldsymbol{u}, \boldsymbol{v} \rangle = \langle \boldsymbol{v}, \boldsymbol{u} \rangle^*$
2. $\langle \boldsymbol{u}, a\boldsymbol{v}_1 + b\boldsymbol{v}_2 \rangle = a\langle \boldsymbol{u}, \boldsymbol{v}_1 \rangle + b\langle \boldsymbol{u}, \boldsymbol{v}_2 \rangle$
   $\langle a\boldsymbol{u}_1 + b\boldsymbol{u}_2, v \rangle = a^*\langle \boldsymbol{v}, \boldsymbol{u}_1 \rangle^* + b^*\langle \boldsymbol{v}, \boldsymbol{u}_2 \rangle^* = a^*\langle \boldsymbol{u}_1, \boldsymbol{v} \rangle + b^*\langle \boldsymbol{u}_2, \boldsymbol{v} \rangle$
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.

$$C_{ij} = \sum_k A_{ik} B_{kj} = A_{ik} B_{kj} \tag{6}$$

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, indices may appear only once, twice or not at all.
2. An 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. An index that appears twice is summed over. It is called a *dummy index*.

1.2.2 Levi-Civita Symbol

The Levi-Civita symbol has three indices and is defined as

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

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

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

A useful identity involving the contraction of two alternating tensors is

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

Example. Prove the vector identity $\boldsymbol{a} \times (\boldsymbol{b} \times \boldsymbol{c}) = (\boldsymbol{a} \cdot \boldsymbol{c})\boldsymbol{b} - (\boldsymbol{a} \cdot \boldsymbol{b})\boldsymbol{c}$.

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

1.2.3 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

$$R^T R = RR^T = \mathbb{1} \quad \Leftrightarrow \quad R^T = R^{-1} \tag{11}$$

1.2.4 Eigenvalues, Eigenvectors and Diagonalization

An eigenvalue equation takes the form

$$\mathbf{A}\boldsymbol{x} = \lambda\boldsymbol{x} \quad \Leftrightarrow \quad A_{ij}x_j = \lambda x_i \tag{12}$$

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

$$(A_{ij} - \lambda\delta_{ij})x_j = 0 \tag{13}$$

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

$$\det(\mathbf{A} - \lambda\mathbb{1}) = 0 \tag{14}$$

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

$$A_{ij}e_j^{(a)} = \lambda_a e_i^{(a)} \tag{15}$$

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

$$\mathbf{M}^\dagger\mathbf{A}\mathbf{M} = \begin{pmatrix}\lambda_1 & & 0\\ & \ddots & \\ 0 & & \lambda_n\end{pmatrix} \tag{16}$$

1.3 Transformations under Rotations

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

$$x'_i = L_{ij}x_j \tag{17}$$

Recall that orthogonality means

$$L_{ij}L_{ik} = L_{ji}L_{ki} = \delta_{jk} \tag{18}$$

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

$$\boldsymbol{e}'^{(i)} = L_{ij}\boldsymbol{e}^{(j)} \quad \Leftrightarrow \quad \boldsymbol{e}^{(i)} = L_{ji}\boldsymbol{e}'^{(j)} \tag{19}$$

Definition.

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

$$\phi(x) \to \phi'(x') = \phi(x) \tag{20}$$

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

$$v_i(x) \to v'_i(x') = L_{ij}v_j(x) \tag{21}$$

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

$$T_{ij}(x) \to T'_{ij}(x') = L_{il}L_{jm}T_{lm}(x) \tag{22}$$

For higher rank tensor,

$$\boxed{T'_{ijk\cdots}(x') = L_{ip}L_{jq}L_{kr}\cdots T_{pqr\cdots}(x)} \tag{23}$$

this equation also gives the definition of a tensor.

1.4 Tensor Calculus

First we define the three direction derivatives

$$\boldsymbol{\nabla} = \left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}\right) \tag{24}$$

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

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

$$(\boldsymbol{\nabla}\phi)_i = \partial_i\phi \tag{25}$$

The gradient transforms under rotations

$$\partial_i\phi(x) \to \frac{\partial}{\partial x'_i}\phi'(x') = \frac{\partial}{\partial x'_i}\phi(x) = \frac{\partial x_p}{\partial x'_i}\frac{\partial}{\partial x_p}\phi(x) = L_{ip}\partial_p\phi(x) \tag{26}$$

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

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

$$\boldsymbol{\nabla} \cdot \boldsymbol{F} = \partial_i F_i \tag{27}$$

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

$$(\boldsymbol{\nabla} \times \boldsymbol{F})_i = \varepsilon_{ijk} \partial_j F_k \tag{28}$$

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

$$\mathcal{L}_x[y(x)] = \left[\frac{\mathrm{d}}{\mathrm{d}x^2} + p(x)\frac{\mathrm{d}}{\mathrm{d}x} + q(x)\right] y(x) = f(x) \tag{29}$$

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

$$y(x) = ay_1(x) + by_2(x) \tag{30}$$

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

$$y(x) = ay_1(x) + by_2(x) + y_0(x) \tag{31}$$

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

$$y_0(x) = u(x)y_1(x) + v(x)y_2(x) \tag{32}$$

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

$$\boxed{u'y_1 + v'y_2 = 0} \tag{33}$$

Rewrite the ODE

$$\begin{aligned}\mathcal{L}_x[y_0(x)] =&u''y_1 + 2u'y_1' + uy_1'' + v''y_2 + 2v'y_2' + vy_2'' \\ &+ p(u'y_1 + uy_1' + v'y_2 + vy_2') + q(uy_1 + vy_2) \\ =&u(y_1'' + py_1' + qy_1) + v(y_2'' + py_2' + qy_2) \\ &+ u''y_1 + 2u'y_1' + v''y_2 + 2v'y_2' + p(u'y_1 + v'y_2) \\ =&u''y_1 + 2u'y_1' + v''y_2 + 2v'y_2' \\ =&u'y_1' + v'y_2' = f\end{aligned} \tag{34}$$

gives

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

So we have

$$\begin{cases} u'y_1 + v'y_2 = 0 \\ u'y_1' + v'y_2' = f \end{cases} \quad \Rightarrow \quad \begin{pmatrix} y_1 & y_2 \\ y_1' & y_2' \end{pmatrix} \begin{pmatrix} u' \\ v' \end{pmatrix} = \mathbf{M} \begin{pmatrix} u' \\ v' \end{pmatrix} = \begin{pmatrix} 0 \\ f \end{pmatrix} \tag{36}$$

then

$$\begin{pmatrix} u' \\ v' \end{pmatrix} = \mathbf{M}^{-1} \begin{pmatrix} 0 \\ f \end{pmatrix} = \frac{1}{W(x)} \begin{pmatrix} y_2' & -y_2 \\ -y_1' & y_1' \end{pmatrix} \begin{pmatrix} 0 \\ f \end{pmatrix} \tag{37}$$

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

$$W(x) = \det(\mathbf{M}) = y_1 y_2' - y_2 y_1' \tag{38}$$

So the solutions are

$$u'(x) = -\frac{y_2(x)f(x)}{W(x)}, \qquad v'(x) = \frac{y_1(x)f(x)}{W(x)} \tag{39}$$

2.2.1 Homogeneous Initial Conditions

The boundary conditions $y(\alpha) = y'(\alpha) = 0$ are called *homogeneous initial conditions*. Integrating eqn.(39) gives

$$u(x) = -\int_\alpha^x \mathrm{d}\tilde{x} \frac{y_2(\tilde{x})f(\tilde{x})}{W(\tilde{x})}, \qquad v(x) = \int_\alpha^x \mathrm{d}\tilde{x} \frac{y_1(\tilde{x})f(\tilde{x})}{W(\tilde{x})} \tag{40}$$

then

$$y_0(x) = u(x)y_1(x) + v(x)y_2(x) = \int_\alpha^x \mathrm{d}\tilde{x} \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) \tag{41}$$

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

$$\begin{aligned} y_0(x) &= \int_\alpha^x \mathrm{d}\tilde{x} \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) + \int_x^\beta \mathrm{d}\tilde{x} \cdot 0 \\ &= \int_\alpha^\beta G(x,\tilde{x}) f(\tilde{x}) \mathrm{d}\tilde{x} \end{aligned} \tag{42}$$

where we have defined the *Green Function*

$$G(x,\tilde{x}) = \begin{cases} 0, & x < \tilde{x} \\ \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})}, & x > \tilde{x} \end{cases} \tag{43}$$

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

$$Y(x) = y(x) - g(x) \tag{44}$$

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

$$F(x) = f(x) - \mathcal{L}_x g(x) = f(x) - g''(x) - p(x)g'(x) - q(x)g(x) \tag{45}$$

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

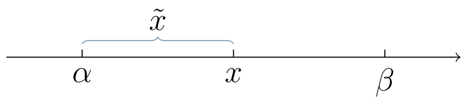

Figure 1: The range of variable x in the problem is $x \in [\alpha, \beta]$.

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

$$y(x) = \int_\alpha^x \mathrm{d}\tilde{x} \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) + a y_1(x) + b y_2(x) \tag{46}$$

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

$$y(\alpha) = b y_2(\alpha) = 0 \quad \Rightarrow \quad b = 0 \tag{47}$$

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

$$y(\beta) = -\int_\alpha^\beta \mathrm{d}\tilde{x} \frac{y_1(\beta)y_2(\tilde{x})}{W(\tilde{x})} f(\tilde{x}) + a y_1(\beta) = 0 \quad \Rightarrow \quad a = \int_\alpha^\beta \mathrm{d}\tilde{x} \frac{y_2(\tilde{x})}{W(\tilde{x})} f(\tilde{x}) \tag{48}$$

which may be substituted into the solution eqn.(46) to give

$$\begin{aligned} y(x) &= \int_\alpha^x \mathrm{d}\tilde{x} \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) + \int_\alpha^\beta \mathrm{d}\tilde{x} \frac{y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) \\ &= \int_\alpha^x \mathrm{d}\tilde{x} \frac{y_1(\tilde{x})y_2(x)}{W(\tilde{x})} f(\tilde{x}) + \int_x^\beta \mathrm{d}\tilde{x} \frac{y_2(\tilde{x})y_1(x)}{W(\tilde{x})} f(\tilde{x}) \\ &= \int_\alpha^\beta \mathrm{d}\tilde{x} G(x, \tilde{x}) f(\tilde{x}) \end{aligned} \tag{49}$$

where we have defined the *Green Function*

$$G(x, \tilde{x}) = \begin{cases} \frac{y_1(\tilde{x})y_2(x)}{W(\tilde{x})}, & \alpha \le \tilde{x} < x \\ \frac{y_2(\tilde{x})y_1(x)}{W(\tilde{x})}, & x < \tilde{x} \le \beta \end{cases} \tag{50}$$

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 $x \neq \tilde{x}$
$$\mathcal{L}_x[G(x, \tilde{x})] = 0 \tag{51}$$
2. $G(x, \tilde{x})$ is continuous at $x = \tilde{x}$
$$\lim_{x \to \tilde{x}_-} G(x, \tilde{x}) = \lim_{x \to \tilde{x}_+} G(x, \tilde{x}) \tag{52}$$
3. $\frac{\partial}{\partial x} G(x, \tilde{x})$ has a unit discontinuity at $x = \tilde{x}$
$$\lim_{x \to \tilde{x}_+} \frac{\partial G(x, \tilde{x})}{\partial x} = 1 + \lim_{x \to \tilde{x}_-} \frac{\partial G(x, \tilde{x})}{\partial x} \tag{53}$$

2.4 Green Function More Generally

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

$$\boxed{\mathcal{L}_x[G(x,\tilde{x})] = \delta(x-\tilde{x})} \tag{54}$$

$\delta(x)$ 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.(54), 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

$$\boxed{y_0(x) = \int_\alpha^\beta \mathrm{d}\tilde{x} G(x,\tilde{x}) f(\tilde{x})} \tag{55}$$

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.

$$\mathcal{L}_x[y_0] = \int_\alpha^\beta \mathrm{d}\tilde{x}\mathcal{L}_x[G(x,\tilde{x})]f(\tilde{x}) = \int_\alpha^\beta \mathrm{d}\tilde{x}\delta(x-\tilde{x})f(\tilde{x}) = f(x) \tag{56}$$

$f(x)$ 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

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

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

$$y(x) = \int_\alpha^\beta \mathrm{d}\tilde{x} G(x,\tilde{x}) f(\tilde{x}) \tag{58}$$

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 $x < \tilde{x}$
$$G(x,\tilde{x}) = 0 \tag{59}$$
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 $y_2(x)$
$$G(x,\tilde{x}) = A(\tilde{x})y_1(x) + B(\tilde{x})y_2(x) \tag{60}$$
We can find A and B by using the properties of G:
   (i) G is continuous at $x = \tilde{x}$
$$A(\tilde{x})y_1(\tilde{x}) + B(\tilde{x})y_2(\tilde{x}) = 0 \tag{61}$$
   (ii) G' has a unit discontinuity at $x = \tilde{x}$
$$A(\tilde{x})y_1'(\tilde{x}) + B(\tilde{x})y_2'(\tilde{x}) = 1 \tag{62}$$
The solution is
$$A(\tilde{x}) = -\frac{y_x(\tilde{x})}{W(\tilde{x})}, \qquad B(\tilde{x}) = \frac{y_1(\tilde{x})}{W(\tilde{x})} \tag{63}$$
where W is the Wronskian of y_1 and y_2.

So we have
$$G(x,\tilde{x}) = \begin{cases} 0, & x < \tilde{x} \\ \frac{y_1(\tilde{x})y_2(x) - y_2(\tilde{x})y_1(x)}{W(\tilde{x})}, & x > \tilde{x} \end{cases} \tag{64}$$
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
$$G(\alpha,\tilde{x}) = G(\beta,\tilde{x}) = 0 \tag{65}$$
We assume y_1 and y_2 are linear independent solutions of homogeneous equation, and we choose $y_1(\alpha) = y_2(\beta) = 0$.
$$G(x,\tilde{x}) = \begin{cases} A(\tilde{x})y_1(x) + B(\tilde{x})y_2(x), & \alpha < x < \tilde{x} \\ C(\tilde{x})y_1(x) + D(\tilde{x})y_2(x), & \tilde{x} < x < \beta \end{cases} \tag{66}$$

1. Boundary conditions: $G(\alpha,\tilde{x}) = G(\beta,\tilde{x}) = 0$
$$A(\tilde{x})y_1(\alpha) + B(\tilde{x})y_2(\alpha) = B(\tilde{x})y_2(\alpha) = 0 \quad \Rightarrow \quad B(\tilde{x}) = 0 \tag{67}$$
$$C(\tilde{x})y_1(\beta) + D(\tilde{x})y_2(\beta) = C(\tilde{x})y_1(\beta) = 0 \quad \Rightarrow \quad C(\tilde{x}) = 0 \tag{68}$$
so we have
$$G(x,\tilde{x}) = \begin{cases} A(\tilde{x})y_1(x), & \alpha < x < \tilde{x} \\ D(\tilde{x})y_2(x), & \tilde{x} < x < \beta \end{cases} \tag{69}$$

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

$$A(\tilde{x})y_1(\tilde{x}) - D(\tilde{x})y_2(\tilde{x}) = 0 \tag{70}$$

$$A(\tilde{x})y_1'(\tilde{x}) - D(\tilde{x})y_2'(\tilde{x}) = 1 \tag{71}$$

so we have

$$A(\tilde{x}) = \frac{y_2(\tilde{x})}{W(\tilde{x})}, \qquad D(\tilde{x}) = \frac{y_1(\tilde{x})}{W(\tilde{x})} \tag{72}$$

The final result

$$G(x, \tilde{x}) = \begin{cases} \frac{y_2(\tilde{x})y_1(x)}{W(\tilde{x})}, & \alpha < x < \tilde{x} \\ \frac{y_1(\tilde{x})y_2(x)}{W(\tilde{x})}, & \tilde{x} < x < \beta \end{cases} \tag{73}$$

which agrees with that calculated before.

2.4.3 Higher Dimensions, More Variables

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

$$\mathcal{L}[y] = f(x_1, x_2, x_3) \tag{74}$$

and

$$\mathcal{L}[G(\boldsymbol{x}, \tilde{\boldsymbol{x}})] = \delta^{(3)}(\boldsymbol{x} - \tilde{\boldsymbol{x}}) = \delta(x_1 - \tilde{x}_1)\delta(x_2 - \tilde{x}_2)\delta(x_3 - \tilde{x}_3) \tag{75}$$

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

$$\int_R \mathrm{d}\tilde{\boldsymbol{x}}\delta^{(3)}(\boldsymbol{x} - \tilde{\boldsymbol{x}})f(\tilde{\boldsymbol{x}}) = \begin{cases} f(\boldsymbol{x}), & \boldsymbol{x} \in R \\ 0, & \boldsymbol{x} \notin R \end{cases} \tag{76}$$

Example. The most famous example is

$$\mathcal{L} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \nabla^2 \tag{77}$$

and the Green function satisfies

$$\nabla^2 G(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = \delta(\boldsymbol{x} - \tilde{\boldsymbol{x}}) \tag{78}$$

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

$$\nabla^2 \phi(\boldsymbol{x}) = 2\pi G\rho \tag{79}$$

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

$$G(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = -\frac{1}{4\pi|\boldsymbol{x} - \tilde{\boldsymbol{x}}|} \tag{80}$$

3 Hilbert Space and Sturm-Liouville Theory

3.1 Hilbert Space

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

$$\langle f, g\rangle = \int_a^b f^*(x)g(x)\mathrm{d}x \tag{81}$$

   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

$$f(x) = \sum_{i=1}^{\infty} f_i y_i(x), \quad f_i \in \mathbb{C} \tag{82}$$

   Then we have

$$\langle y_k, f\rangle = \langle y_k, \sum_{i=1}^{\infty} f_i y_i\rangle = \sum_{i=1}^{\infty} f_i\langle y_k, y_i\rangle = \sum_{i=1}^{\infty} f_i\delta_{ik} = f_k \tag{83}$$

3.2 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**.

3.2.1 Self-Adjoint Differential Operators

Consider the differential operator

$$\boxed{\mathcal{L} = -\frac{\mathrm{d}}{\mathrm{d}x}\left[\rho(x)\frac{\mathrm{d}}{\mathrm{d}x}\right] + \sigma(x)} \tag{84}$$

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].

$$\mathcal{L}y = -\frac{\mathrm{d}}{\mathrm{d}x}\left(\rho\frac{\mathrm{d}y}{\mathrm{d}x}\right) + \sigma y = -(\rho y')' + \sigma y \tag{85}$$

[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.

Definition. *A second order linear differential operator $\mathcal{L}$ is self-adjoint on Hilbert space $\mathcal{H}$ if* [2]

$$\boxed{\langle u, \mathcal{L}v\rangle = \langle v, \mathcal{L}u\rangle^*, \quad \forall u, v \in \mathcal{H}} \tag{86}$$

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

$$\begin{aligned}
\langle u, \mathcal{L}v\rangle &= \int_a^b u^* \left[-(\rho v')' + \sigma v\right] \mathrm{d}x \\
&= - \left. u^* \rho v' \right|_a^b + \int_a^b \left(u^{*\prime} \rho v' + u^* \sigma v\right) \mathrm{d}x \\
&= - \left. u^* \rho v' \right|_a^b + \left. u^{*\prime} \rho v \right|_a^b + \int_a^b \left(-(u^{*\prime}\rho)' v + u^* \sigma v\right) \mathrm{d}x \\
&= \left. (-u^* \rho v' + u^{*\prime} \rho v) \right|_a^b + \int_a^b \left(-(u^{*\prime}\rho)' + u^* \sigma\right) v \mathrm{d}x \\
&= \left. (-u^* \rho v' + u^{*\prime} \rho v) \right|_a^b + \left[\int_a^b \left(-(u'\rho)' + u \sigma\right) v^* \mathrm{d}x\right]^* \\
&= \left. (-u^* \rho v' + u^{*\prime} \rho v) \right|_a^b + \langle v, \mathcal{L}u\rangle^*
\end{aligned} \tag{87}$$

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

$$\boxed{\rho \left[u^{*\prime} v - u^* v'\right]_a^b = 0} \tag{88}$$

3.2.2 Weight Functions

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

$$\tilde{\mathcal{L}} = -\frac{\mathrm{d}}{\mathrm{d}x}\left(A(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) - B(x)\frac{\mathrm{d}}{\mathrm{d}x} + C(x) \tag{89}$$

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.*

$$w(x)\left[-(Ay')' - By' + Cy\right] = -(\rho y')' + \sigma y \tag{90}$$

rearranging this

$$-w(Ay')' - Bwy' + Cwy = -(\rho y')' + \sigma y \tag{91}$$

so we have

$$\begin{cases} Awy'' = \rho y'' \\ A'wy' - Bwy' = \rho' y' \\ Cwy = \sigma y \end{cases} \tag{92}$$

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

then

$$\frac{w'}{w} = \frac{B}{A}, \qquad Aw = \rho, \qquad Cw = \sigma \tag{93}$$

We choose $w(x)$ such that

$$w(x) = \exp\left[\int_a^x \frac{B(\tilde{x})}{A(\tilde{x})}\mathrm{d}\tilde{x}\right] \tag{94}$$

where $w(a) = 1$.

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

$$\langle f, g\rangle_w = \langle f, wg\rangle = \int_a^b f^*(x)w(x)g(x)\mathrm{d}x = \langle wf, g\rangle \tag{95}$$

3.2.3 Eigenfunctions and Eigenvalues

Consider the inhomogeneous eigenfunction equation

$$\tilde{\mathcal{L}}y = \lambda y \tag{96}$$

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

$$\boxed{\mathcal{L}y = \lambda wy} \tag{97}$$

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

$$\begin{aligned}\langle y_i, \mathcal{L}y_j\rangle =& \langle y_j, \mathcal{L}y_i\rangle^* = \lambda_i^*\langle y_j, \omega y_i\rangle^* = \lambda_i^*\langle y_i, \omega y_j\rangle = \lambda_i^*\langle y_i, y_j\rangle_w \\ =& \lambda_j\langle y_i, wy_j\rangle = \lambda_j\langle y_i, y_j\rangle_w\end{aligned} \tag{98}$$

Compare the two expressions at the end of each line, we find

$$(\lambda_i^* - \lambda_j)\langle y_i, y_j\rangle_w = 0 \tag{99}$$

- For $i = j$ we have
  $$(\lambda_i^* - \lambda_i)\|y_i\|_w^2 = 0 \tag{100}$$
  so, if we have non-zero eigenfunctions, then $\lambda_i^* = \lambda_i$, *i.e.*, the eigenvalues are real.

- For $i \neq j$ we have
  $$(\lambda_i - \lambda_j)\langle y_i, y_j\rangle_w = 0 \tag{101}$$
  so, if we are considering distinct eigenvalues, then $\langle y_i, y_j\rangle_w = 0$, *i.e.*, the eigenfunctions are orthogonal with weight $w(x)$.

□

3.2.4 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

$$g(x) = \sum_n g_n f_n(x), \quad g_n \in \mathbb{C} \tag{102}$$

where

$$\boxed{g_n = \langle f_n, g \rangle_\omega = \int_a^b f_n^*(x) w(x) g(x) \mathrm{d}x} \tag{103}$$

Substituting into the expansion we find

$$\begin{aligned} g(x) &= \sum_n \int_a^b \mathrm{d}\tilde{x} \left[f_n^*(\tilde{x}) w(\tilde{x}) g(\tilde{x}) \right] f_n(x) \\ &= \int_a^b \mathrm{d}\tilde{x} g(\tilde{x}) \left[w(\tilde{x}) \sum_n f_n(x) f_n^*(\tilde{x}) \right] \\ &= \int_a^b \mathrm{d}\tilde{x} \delta(x - \tilde{x}) g(\tilde{x}) \end{aligned} \tag{104}$$

where

$$\delta(x - \tilde{x}) = w(\tilde{x}) \sum_n f_n(\tilde{x}) f_n^*(\tilde{x}) \tag{105}$$

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

$$\begin{aligned} \int_a^b |u|^2 \omega \mathrm{d}x =& \langle u, u \rangle_w = \langle \sum_n u_n f_n(x), \sum_m u_m f_m(x) \rangle_w \\ =& \sum_{n,m} u_n^* u_m \langle f_n, f_m \rangle_w = \sum_{n,m} u_n^* u_m \delta_{nm} = \sum_n |u_n|^2 \end{aligned} \tag{106}$$

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

$$\langle u, u \rangle_w = \sum_n |u_n|^2 \tag{107}$$

3.2.5 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

$$\boxed{G(x, \tilde{x}) = \sum_n \frac{y_n(x) y_n^*(\tilde{x})}{\lambda_n}, \qquad \lambda_n \neq 0} \tag{108}$$

Proof.

$$
\begin{aligned}
\mathcal{L}_x[G(x,\tilde{x})] &= \sum_n \frac{\mathcal{L}_x[y_n(x)]y_n^*(\tilde{x})}{\lambda_n} \\
&= \sum_n w(x)y_n(x)y_n^*(\tilde{x}) \\
&= \frac{\omega(x)}{\omega(\tilde{x})}\left[\omega(\tilde{x})\sum_n y_n(x)y_n^*(\tilde{x})\right] \\
&= \delta(x-\tilde{x})
\end{aligned} \tag{109}
$$

□

3.2.6 Eigenfunction Expansions for Solving ODEs

As an example, consider the differential equation

$$
\mathcal{L}y - \nu y = f \tag{110}
$$

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

$$
y(x) = \sum_n a_n y_n(x), \qquad f(x) = \sum_n f_n y_n(x) \tag{111}
$$

Substituting into the original equation, we find

$$
\mathcal{L}\sum_n a_n y_n - \nu \sum_n a_n y_n = \sum_n (a_n\lambda_n - \nu a_n)y_n = \sum_n f_n y_n \tag{112}
$$

So that

$$
a_n = \frac{f_n}{\lambda_n - \nu}, \qquad (\lambda_n \neq \nu) \tag{113}
$$

so that the solution is given by

$$
\begin{aligned}
y(x) &= \sum_n \frac{f_n}{\lambda_n - \nu} y_n(x) = \sum_n \frac{\langle y_n, f\rangle}{\lambda_n - \nu} y_n(x) \\
&= \int_a^b \mathrm{d}x' \sum_n \frac{y_n(x)y_n^*(x')}{\lambda_n - \nu} f(x') \\
&= \int_a^b \mathrm{d}x' G(x,x') f(x')
\end{aligned} \tag{114}
$$

hence the Green function of the problem as

$$
G(x,x') = \sum_n \frac{y_n(x)y_n^*(x')}{\lambda_n - \nu} \tag{115}
$$

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

3.3 Legendre Polynomials

3.3.1 Examples

Example. The two examples differ only by boundary conditions.

(1) Let

$$\mathcal{L} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \qquad x \in [0, 2\pi R] \tag{116}$$

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

$$-y_n'' = \lambda_n y_n \tag{117}$$

and the eigenfunctions and the corresponding eigenvalues are

$$y_n = \sin\left(\frac{n}{2R}x\right), \qquad \lambda_n = \left(\frac{n}{2R}\right)^2, \qquad n = 1, 2, 3, \cdots \tag{118}$$

(2) Let

$$\mathcal{L} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \qquad x \in [0, 2\pi R] \tag{119}$$

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

$$-y_m'' = \lambda_m y_m \tag{120}$$

and the eigenfunctions and the corresponding eigenvalues are

$$y_m = \exp\left(i\frac{m}{R}x\right), \qquad \lambda_m = \left(\frac{m}{2R}\right)^2, \qquad m \in \mathbb{Z} \tag{121}$$

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

3.3.2 Legendre's Equation

Legendre's equation

$$(1 - x^2)y'' - 2xy' + l(l+1)y = 0 \quad \text{with} \quad x \in [-1, 1] \tag{122}$$

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

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

or

$$\mathcal{L}y = l(l+1)y \tag{124}$$

where

$$\mathcal{L} = -\frac{\mathrm{d}}{\mathrm{d}x}\left[(1-x^2)\frac{\mathrm{d}}{\mathrm{d}x}\right] \tag{125}$$

is self-adjoint on a Hilbert space of functions that are finite at ± 1. Assume that eigenfunctions of eqn.(123) are polynomials

$$y_n(x) = x^{m_n} + a_{m_n-1}x^{m_n-1} + \cdots + a_1 x + a_0 \tag{126}$$

Substituting the polynomial solution y_n into eqn.(123), then thinking about equation coefficients of partial of x. The highest power m_n satisfies the relation

$$m_n(m_n+1) = \lambda \tag{127}$$

So eigenvalues take form

$$\lambda = l(l+1), \qquad l \in \mathbb{N} \tag{128}$$

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

$$\int_{-1}^{1} y_l^*(x) y_{l'}(x) = \delta_{ll'} \tag{129}$$

3.4 Spherical Harmonics

Laplace's equation in spherical coordinates is given by

$$\nabla^2 f(r,\theta,\phi) = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin\theta}\frac{\partial^2 f}{\partial\phi^2} \tag{130}$$

Ansatz

$$f(r,\theta,\phi) = r^l \mathrm{e}^{im\phi}\Theta(\theta) \tag{131}$$

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

$$l(l+1)\mathrm{e}^{im\phi}\Theta(\theta) + \frac{\mathrm{e}^{im\phi}}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) - \frac{\Theta}{\sin\theta}m^2\mathrm{e}^{im\phi} = 0 \tag{132}$$

Rearrange this, we have

$$\sin^2\theta\, l(l+1) + \frac{\sin\theta}{\Theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) = m^2 \tag{133}$$

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

$$\frac{\mathrm{d}}{\mathrm{d}\theta} = \frac{\mathrm{d}}{\mathrm{d}u}\frac{\mathrm{d}u}{\mathrm{d}\theta} = -\sin\theta\frac{\mathrm{d}}{\mathrm{d}u} \tag{134}$$

Then the equation becomes self-adjoint form

$$-[(1-u^2)P']' + \frac{m^2}{1-u^2}P = l(l+1)P \tag{135}$$

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

$$\int_{-1}^{1} P_l^m(u)P_{l'}^m(u)\mathrm{d}u = \frac{2(l+m)!}{(2l+1)(l-m)}\delta_{ll'} \tag{136}$$

Similarly, the equation can be expressed as

$$-[(1-u^2)P']' - l(l+1)P = -\frac{m^2}{1-u^2}P \tag{137}$$

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

$$\int_{-1}^{1} \frac{P_l^m(u)P_l^{m'}(u)}{1-u^2}\mathrm{d}u = \frac{(l+m)!}{m(l-m)}\delta_{mm'} \tag{138}$$

Finally we get

$$Y_l^m = (-1)^m\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)\mathrm{e}^{im\phi}, \quad l \in \mathbb{N},\ -l \le m \le l \tag{139}$$

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

$$\delta_{ll'}\delta_{mm'} = \int_0^{2\pi}\int_0^{\pi} Y_l^m(\theta,\phi)Y_{l'}^{m'}(\theta,\phi)\sin\theta\mathrm{d}\theta\mathrm{d}\phi \tag{140}$$

So any function f can be expressed as

$$f(\theta,\phi) = \sum_l \sum_{m=-l}^{l} f_{lm}Y_l^m(\theta,\phi) \tag{141}$$

where

$$f_{lm} = \int_{\mathbf{S}^2} Y_l^{*m} f\mathrm{d}\Omega \tag{142}$$

4 Integral Transforms

4.1 Fourier Series

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

$$f(x) = \sum_{n=-\infty}^{\infty} f_n y_n(x), \qquad f_n \in \mathbb{C} \tag{143}$$

We choose the Fourier basis

$$y_n(x) = \frac{1}{\sqrt{2\pi R}} \mathrm{e}^{inx/R} \tag{144}$$

with the orthogonality

$$\langle y_n, y_m \rangle = \int_0^{2\pi R} y_n^* y_m \mathrm{d}x = \delta_{nm} \tag{145}$$

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

$$\begin{aligned} f_n &= \int_{-\pi R}^{\pi R} y_n^*(x) f(x) \mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi R}} \int_{-\pi R}^{\pi R} \mathrm{e}^{-inx/R} f(x) \mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi R}} \int_{-\pi R}^{\pi R} \mathrm{e}^{-ik_n x} f(x) \mathrm{d}x \end{aligned} \tag{146}$$

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

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} f(x) \mathrm{d}x \tag{147}$$

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*

$$\boxed{\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \mathrm{e}^{-ikx} \mathrm{d}x} \tag{148}$$

The inverse Fourier transform is defined as

$$\boxed{f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) \mathrm{e}^{ikx} \mathrm{d}k} \tag{149}$$

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

$$\mathcal{F}^{-1}[\mathcal{F}[f]] = f \quad \Rightarrow \quad \mathcal{F}^{-1}\mathcal{F} = \mathbb{1} \tag{150}$$

4.2.2 Dirac Delta-Function

$$\begin{aligned}
f(x) =& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) \mathrm{e}^{ikx} \mathrm{d}k \\
=& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x') \mathrm{e}^{-ikx'} \mathrm{d}x' \right] \mathrm{e}^{ikx} \mathrm{d}k \\
=& \int_{-\infty}^{\infty} f(x') \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{ik(x-x')} \mathrm{d}k \right] \mathrm{d}x' \\
=& \int_{-\infty}^{\infty} f(x') \delta(x-x') \mathrm{d}x'
\end{aligned} \tag{151}$$

where we have defined the *Dirac delta-function*

$$\boxed{\delta(x-x') = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{ik(x-x')} \mathrm{d}k} \tag{152}$$

4.2.3 Properties of the Fourier Transform

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

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

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

$$\tilde{f}^*(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-iky} f(-y) \mathrm{d}(-y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-iky} f(y) \mathrm{d}y = \tilde{f}(k) \tag{154}$$

□

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

$$\tilde{f}^*(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-iky} f(-y) \mathrm{d}(-y) = -\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-iky} f(y) \mathrm{d}y = -\tilde{f}(k) \tag{155}$$

□

2. Differentiation

$$\mathcal{F}[f^{(n)}(x)] = (ik)^n \tilde{f}(k) \tag{156}$$

Proof. Consider the first order derivative

$$\begin{aligned}
\mathcal{F}[f'(x)] =& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{-ikx} f'(x) \\
=& \frac{1}{\sqrt{2\pi}} \left[f(x) \mathrm{e}^{-ikx} \right]_{-\infty}^{\infty} - \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x f(x) (-ik) \mathrm{e}^{-ikx} \\
=& ik\tilde{f}(k)
\end{aligned} \tag{157}$$

Repeat the process so we can prove the relation. □

3. Multiplication by x

$$\mathcal{F}[xf(x)] = i\frac{\mathrm{d}}{\mathrm{d}x}\tilde{f}(k) \tag{158}$$

$$\mathcal{F}[x^n f(x)] = \left(i\frac{\mathrm{d}}{\mathrm{d}x}\right)^n \tilde{f}(k) \tag{159}$$

4. Rigid shift of coordinate

$$\mathcal{F}[f(x-a)] = \mathrm{e}^{-ika}\tilde{f}(k) \tag{160}$$

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

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

□

4.2.4 Parseval's Theorem

Parseval's theorem for Fourier transforms states that

$$\boxed{\int_{-\infty}^{\infty} |f(x)|^2\mathrm{d}x = \int_{-\infty}^{\infty} |\tilde{f}(k)|^2\mathrm{d}k} \tag{162}$$

Proof.

$$\begin{aligned}\int_{-\infty}^{\infty} |f(x)|^2\mathrm{d}x =& \int_{-\infty}^{\infty} f(x)f^*(x)\mathrm{d}x \\ =& \frac{1}{2\pi}\int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty}\mathrm{d}k\int_{-\infty}^{\infty}\mathrm{d}k'\tilde{f}(k)\tilde{f}^*(k')\mathrm{e}^{i(k-k')x}\right]\mathrm{d}x \\ =& \int_{-\infty}^{\infty}\mathrm{d}k\int_{-\infty}^{\infty}\mathrm{d}k'\tilde{f}(k)\tilde{f}^*(k')\left[\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{e}^{i(k-k')x}\mathrm{d}x\right] \\ =& \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\tilde{f}(k)\tilde{f}^*(k')\delta(k-k')\mathrm{d}k\mathrm{d}k' \\ =& \int_{-\infty}^{\infty}\tilde{f}(k)\tilde{f}^*(k)\mathrm{d}k = \int_{-\infty}^{\infty}|\tilde{f}(k)|^2\mathrm{d}k\end{aligned} \tag{163}$$

□

4.2.5 Convolution Theorem

Theorem.

$$\boxed{(f * g)(x) = \int_{-\infty}^{\infty} f(y)g(x-y)\mathrm{d}y} \tag{164}$$

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.

$$\mathcal{F}(f * g) = \sqrt{2\pi}\tilde{f}(k)\tilde{g}(k) \tag{165}$$

Proof.

$$\begin{aligned}\mathcal{F}[f * g] =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}x\mathrm{e}^{-ikx}\int_{-\infty}^{\infty}\mathrm{d}y f(y)g(x-y) \\ =& \int_{-\infty}^{\infty}\mathrm{d}y\mathrm{e}^{-iky}f(y)\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}(x-y)\mathrm{e}^{-ik(x-y)}g(x-y) \\ =& \int_{-\infty}^{\infty}\mathrm{d}y\mathrm{e}^{-iky}f(y)\tilde{g}(k) = \sqrt{2\pi}\tilde{f}(k)\tilde{g}(k)\end{aligned} \tag{166}$$

□

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

$$\mathcal{F}[f(x)g(x)] = \frac{1}{\sqrt{2\pi}}\tilde{f}(k) * \tilde{g}(k) \tag{167}$$

Proof.

$$\begin{aligned}\mathcal{F}[f(x)g(x)] =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}x\mathrm{e}^{-ikx}f(x)g(x) \\ =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}x\mathrm{e}^{-ikx}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}p\mathrm{e}^{ipx}\tilde{f}(p)\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}q\mathrm{e}^{iqx}\tilde{g}(q) \\ =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}p\mathrm{d}q\tilde{f}(p)\tilde{g}(q)\left[\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}x\mathrm{e}^{-i(k-p-q)x}\right] \\ =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{d}p\mathrm{d}q\tilde{f}(p)\tilde{g}(q)\delta(k-p-q) \\ =& \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}p\tilde{f}(p)\tilde{g}(k-p) \\ =& \frac{1}{\sqrt{2\pi}}\tilde{f}(k) * \tilde{g}(k)\end{aligned} \tag{168}$$

□

4.2.6 Examples of Fourier Transform

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

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-ikx} \mathrm{d}x = \sqrt{2\pi}\delta(k) \tag{169}$$

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

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{ik_0 x} \mathrm{e}^{-ikx} \mathrm{d}x = \sqrt{2\pi}\delta(k - k_0) \tag{170}$$

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

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(x - x_0) \mathrm{e}^{-ikx} \mathrm{d}x = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-ikx_0} \tag{171}$$

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

$$\begin{aligned}
\tilde{f}(k) =& \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma(2\pi)^{1/4}} \int_{-\infty}^{\infty} \mathrm{e}^{-x^2/4\sigma^2} \mathrm{e}^{-ikx} \mathrm{d}x \\
=& \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma(2\pi)^{1/4}} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2}{4\sigma^2} - ikx\right) \mathrm{d}x \\
=& \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma(2\pi)^{1/4}} \int_{-\infty}^{\infty} \exp\left[-\frac{1}{4\sigma^2}\left(x + ik2\sigma\right)^2 - k^2\sigma^2\right] \mathrm{d}x \\
=& \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma(2\pi)^{1/4}} \mathrm{e}^{-k^2\sigma^2} \int_{-\infty}^{\infty} \exp\left[-\frac{1}{4\sigma^2}\left(x + ik2\sigma\right)^2\right] \mathrm{d}x \\
=& \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma(2\pi)^{1/4}} \mathrm{e}^{-k^2\sigma^2} \int_{-\infty}^{\infty} \exp\left(-\frac{1}{4\sigma^2} x'^2\right) \mathrm{d}x' \\
=& \frac{\sqrt{2\sigma}}{(2\pi)^{\frac{1}{4}}} \mathrm{e}^{-k^2\sigma^2}
\end{aligned} \tag{172}$$

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

$$\begin{aligned}
\tilde{f}(k) =& \frac{1}{\sqrt{2\pi}} \int_{-a}^{a} \mathrm{e}^{-ikx} \mathrm{d}x = \frac{1}{\sqrt{2\pi}} \left[-\frac{1}{ik} \mathrm{e}^{-ikx}\right]_{-a}^{a} \\
=& \sqrt{\frac{2}{\pi}} \frac{\sin(ka)}{k} = a\sqrt{\frac{2}{\pi}} \text{sinc}(ak)
\end{aligned} \tag{173}$$

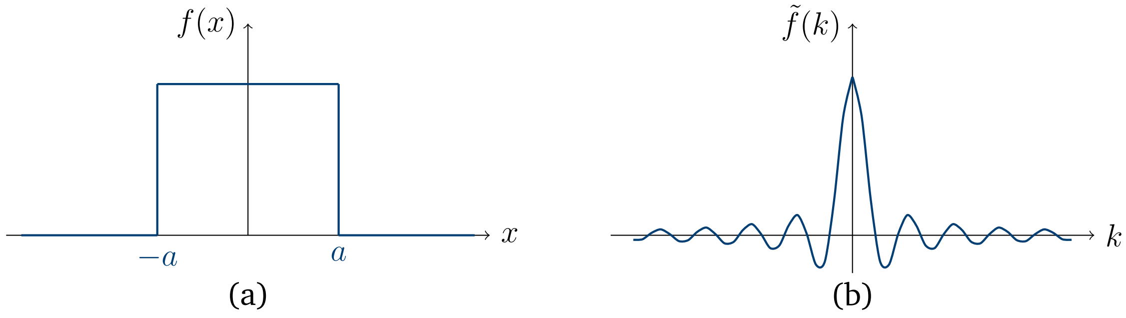

Figure 2: Top-hat function.

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

$$h(x) = \begin{cases} 1 & |x| < \frac{a}{2} \\ 0 & |x| \geq \frac{a}{2} \end{cases} \tag{174}$$

so we have

$$\tilde{h}(k) = \frac{a}{\sqrt{2\pi}} \text{sinc}\left(\frac{ak}{2}\right) \tag{175}$$

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

$$I(x = X) = I\left(k_x = \frac{2\pi X}{\lambda D}\right) = |\tilde{h}(k_x)|^2 = \frac{a^2}{2\pi}\text{sinc}^2\left(\frac{a\pi X}{2\lambda D}\right) \tag{176}$$

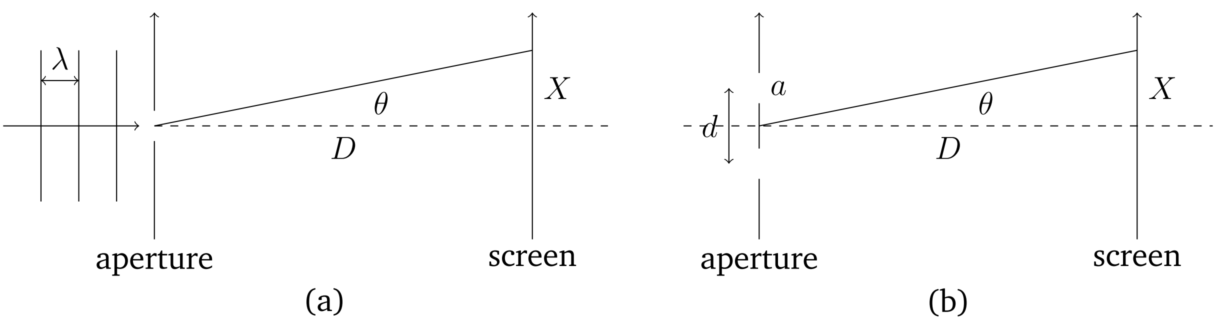

Figure 3: Geometry for Fraunhofer diffraction. (a) Diffraction through an aperture. (b) Double slit diffraction.

4.3.2 Double Slit Diffraction

The aperture function is given by

$$h(x) = f(x)g(x) \tag{177}$$

where

$$f(x) = \delta\left(x - \frac{d}{2}\right) + \delta\left(x + \frac{d}{2}\right) \tag{178}$$

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

$$\begin{aligned}\tilde{f}(k) =& \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}x \mathrm{e}^{-ikx} \left[\delta\left(x - \frac{d}{2}\right) + \delta\left(x + \frac{d}{2}\right)\right] \\ =& \frac{1}{\sqrt{2\pi}} \left(\mathrm{e}^{-ikd/2} + \mathrm{e}^{ikd/2}\right) = \sqrt{\frac{2}{\pi}} \cos\left(\frac{kd}{2}\right)\end{aligned} \tag{179}$$

so we have

$$\begin{aligned}\mathcal{F}(f * g) =& \sqrt{2\pi}\tilde{f}(k)\tilde{g}(k) \\ =& \sqrt{2\pi}\sqrt{\frac{2}{\pi}} \cos\left(\frac{kd}{2}\right) \frac{a}{\sqrt{2\pi}} \mathrm{sinc}\left(\frac{ak}{2}\right) \\ =& \sqrt{\frac{2}{\pi}} a \mathrm{sinc}\left(\frac{ak}{2}\right) \cos\left(\frac{kd}{2}\right)\end{aligned} \tag{180}$$

and the intensity on the screen is given by

$$I(k) = \frac{2a^2}{\pi} \mathrm{sinc}^2\left(\frac{ak}{2}\right) \cos^2\left(\frac{kd}{2}\right) \tag{181}$$

4.3.3 Diffusion Equation

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

$$\frac{\partial \theta}{\partial t} = D \frac{\partial^2 \theta}{\partial x^2} \tag{182}$$

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

$$\frac{\partial}{\partial t}\tilde{\theta}(k,t) = D(ik)^2\tilde{\theta}(k,t) = -Dk^2\tilde{\theta}(k,t) \tag{183}$$

the solution is

$$\tilde{\theta}(k,t) = \tilde{\theta}(k,0)\mathrm{e}^{-Dk^2t} = \mathcal{F}[\delta(x)]\mathrm{e}^{-Dk^2t} = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{-Dk^2t} \tag{184}$$

So we have

$$\begin{aligned}\theta(x,t) =&\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k e^{ikx}\mathrm{e}^{-Dk^2t} \\ =&\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k \exp\left[-Dt\left(k-\frac{ix}{2Dt}\right)^2-\frac{x^2}{4Dt}\right]\mathrm{d}k \\ =&\frac{1}{2\pi}\mathrm{e}^{-x^2/4Dt}\int_{-\infty}^{\infty} e^{-Dtq^2}\mathrm{d}q \\ =&\frac{1}{2\pi}\sqrt{\frac{\pi}{Dt}}\mathrm{e}^{-x^2/4Dt} \qquad \left(\int_{-\infty}^{\infty}\mathrm{e}^{-\alpha x^2}\mathrm{d}x=\sqrt{\frac{\pi}{\alpha}}\right)\end{aligned} \tag{185}$$

Hence the final result

$$\theta(x,t)=\frac{1}{2\sqrt{\pi Dt}}\mathrm{e}^{-x^2/4Dt} \tag{186}$$

4.4 Laplace Transforms

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

$$\mathcal{L}[f(t)]=\hat{f}(s)=\int_0^{\infty}\mathrm{d}t\mathrm{e}^{-st}f(t) \tag{187}$$

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

4.4.1 Properties

(1)

$$\boxed{\mathcal{L}[f'(t)]=s\hat{f}(s)-f(0)} \tag{188}$$

Proof.

$$\begin{aligned}\mathcal{L}[f'(t)]=&\int_0^{\infty}\mathrm{d}t\mathrm{e}^{-st}f'(t) \\ =&\mathrm{e}^{-st}f(t)\big|_0^{\infty}+s\int_0^{\infty}\mathrm{d}t\mathrm{e}^{-st}f(t)=s\hat{f}(s)-f(0)\end{aligned} \tag{189}$$

□

More generally

$$\boxed{\mathcal{L}[f^{(n)}(t)]=s^n\hat{f}(s)-s^{n-1}f(0)-s^{n-2}f'(0)-\cdots-f^{(n-1)}(0)} \tag{190}$$

(2)

$$\boxed{\mathcal{L}[t^nf(t)]=(-1)^n\frac{\mathrm{d}^n}{\mathrm{d}s^n}\hat{f}(s)} \tag{191}$$

Proof.

$$\begin{aligned}(-1)^n\frac{\mathrm{d}^n}{\mathrm{d}s^n}\hat{f}(s) =&(-1)^n\frac{\mathrm{d}^n}{\mathrm{d}s^n}\int_0^\infty \mathrm{d}t\mathrm{e}^{-st}f(t) = (-1)^n\int_0^\infty \mathrm{d}t(-t)^n\mathrm{e}^{-st}f(t)\\ =&\int_0^\infty \mathrm{d}t\mathrm{e}^{-st}t^n f(t) = \mathcal{L}[t^n f(t)]\end{aligned} \tag{192}$$

□

Example. Consider the differential equation

$$f'' + 5f' + 6f = 0 \tag{193}$$

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

$$s^2\hat{f}(s) - sf(0) - f'(0) + 5[s\tilde{f}(s) - f(0)] + 6\tilde{f}(s) = \tilde{f}(s)(s^2+5s+6) = \frac{1}{s} \tag{194}$$

rearranging this, we have

$$\tilde{f}(s) = \frac{1}{s(s+2)(s+3)} = \frac{1}{6s} - \frac{1}{2(s+2)} + \frac{1}{3(s+3)} \tag{195}$$

So

$$f(t) = \frac{1}{6} - \frac{1}{2}\mathrm{e}^{-2t} + \frac{1}{3}\mathrm{e}^{-3t} \tag{196}$$

4.4.2 Convolution Theorem for Laplace Transforms

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

$$f_1 * f_2 = \int_{-\infty}^{\infty} f_1(t')f_2(t-t')\mathrm{d}t' \tag{197}$$

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

$$\boxed{f_1 * f_2 = \int_0^t f_1(t')f_2(t-t')\mathrm{d}t'} \tag{198}$$

Theorem.
The convolution theorem for Laplace transforms

$$\mathcal{L}[f_1 * f_2] = \tilde{f}_1(s)\tilde{f}_2(s) \tag{199}$$

Proof.

$$\begin{aligned}\mathcal{L}[f_1 * f_2] &= \int_0^\infty \mathrm{d}t\mathrm{e}^{-st}\int_0^t f_1(t')f_2(t-t')\mathrm{d}t'\\ &= \int_0^\infty \mathrm{d}t' f_1(t')\int_{t'}^\infty \mathrm{d}t\mathrm{e}^{-st}f_2(t-t')\\ &= \int_0^\infty \mathrm{d}t'\mathrm{e}^{-st'}f_1(t')\int_{t'}^\infty \mathrm{d}t\mathrm{e}^{-s(t-t')}f_2(t-t')\\ &=\tilde{f}_1(s)\tilde{f}_2(s)\end{aligned} \tag{200}$$

□

5 Complex Analysis

5.1 Complex Functions of a Complex Variable

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

$$w = f(z) = u(x, y) + iv(x, y) \tag{201}$$

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

$$z = r\mathrm{e}^{i\theta} \tag{202}$$

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

$$\mathrm{e}^z = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \cdots \tag{203}$$

$$\cos z = 1 - \frac{z^2}{2!} + \frac{z^4}{4!} - \cdots \tag{204}$$

$$\ln(1 + z) = z - \frac{z^2}{2} + \frac{z^3}{3} - \cdots \qquad (|z| < 1) \tag{205}$$

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*

$$\lim_{z\to z_0} f(z) = f(z_0) \tag{206}$$

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

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

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 $z = z_0 + \delta z$

$$\lim_{\delta z \to 0} \frac{(z_0 + \delta z)^2 - z_0^2}{\delta z} = 2z_0 \tag{208}$$

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

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

$f(z) = z^*$ 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.

$$\frac{\partial f}{\partial x} = \frac{\mathrm{d}f}{\mathrm{d}z}\frac{\partial z}{\partial x} = f', \qquad \frac{\partial f}{\partial y} = \frac{\mathrm{d}f}{\mathrm{d}z}\frac{\partial z}{\partial y} = if' \tag{210}$$

which shows

$$i\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y} \quad \Rightarrow \quad i\left(\frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x}\right) = \left(\frac{\partial u}{\partial y} + i\frac{\partial v}{\partial y}\right) \tag{211}$$

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

$$\boxed{\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \qquad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}} \tag{212}$$

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 $v = 2xy$.

$$\frac{\partial u}{\partial x} = 2x, \qquad \frac{\partial u}{\partial y} = -2y \tag{213}$$

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

satisfy the C-R equations.

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

$$\frac{\partial u}{\partial x} = 1 \neq \frac{\partial v}{\partial y} = 0 \tag{215}$$

C-R equations fail.

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

$$\frac{\partial u}{\partial x} = 2x, \qquad \frac{\partial u}{\partial y} = 2y, \qquad \frac{\partial v}{\partial x} = \frac{\partial v}{\partial y} = 0 \tag{216}$$

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 neighhood of z_0.

$$f(z) = c_0 + c_1(z - z_0) + c_2(z - z_0)^2 + \cdots = \sum_{k=0}^{\infty} c_k (z - z_0)^k \tag{217}$$

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

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial x}\frac{\partial u}{\partial x} = \frac{\partial}{\partial x}\frac{\partial v}{\partial y} = \frac{\partial}{\partial y}\frac{\partial v}{\partial x} = -\frac{\partial}{\partial y}\frac{\partial u}{\partial y} = -\frac{\partial^2 u}{\partial y^2} \tag{218}$$

Hence

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \nabla^2 u = 0 \tag{219}$$

$u(x, y)$ 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 $u(x, y) = \cos x \cosh y$

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\cos x \cosh y + \cos x \cosh y = 0 \tag{220}$$

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

$$\frac{\partial v}{\partial y} = \frac{\partial u}{\partial x} = -\sin x \cosh y \quad \Rightarrow \quad v = -\sin x \sinh y + c_1(y) \tag{221}$$

$$\frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y} = -\cos x \sinh y \quad \Rightarrow \quad v = -\sin x \sinh y + c_2(x) \tag{222}$$

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

$$f(z) = \cos x \cosh y - i \sin x \sinh y + \tilde{c} \tag{223}$$

is analytic by construction.

5.3 Multi-Valued Functions

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

$$\begin{cases} F_1(z) = r^{1/3} \mathrm{e}^{i\theta/3} \\ F_2(z) = r^{1/3} \mathrm{e}^{i\theta/3 + 2\pi i/3} \\ F_3(z) = r^{1/3} \mathrm{e}^{i\theta/3 + 4\pi i/3} \end{cases} \tag{224}$$

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

$$f(z) = F_i(z) \qquad \text{on sheet } i \tag{225}$$

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

$$f(z) = \ln r + i\theta + 2\pi i n \tag{226}$$

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) $y = x$.

$$\int_C z\mathrm{d}z = \int_C (x+iy)(\mathrm{d}x + i\mathrm{d}y) = \int_C (x\mathrm{d}x - y\mathrm{d}y) + i\int_C (y\mathrm{d}x + x\mathrm{d}y) \tag{227}$$

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

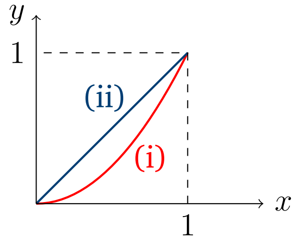

Figure 5: The two paths, (i) $y = x^2$ and (ii) $y = x$, along with the function $f(z)$ is to be integrated in the example.

5.4.2 Cauchy's Theorem

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

$$\oint_C f(z)\mathrm{d}z = 0 \tag{228}$$

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

$$\oint_C (P\mathrm{d}x + Q\mathrm{d}y) = \iint_D \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y}\right) \mathrm{d}x\mathrm{d}y \tag{229}$$

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

$$\begin{aligned}
\oint_C f(z)\mathrm{d}z &= \oint_C (u(x,y) + iv(x,y))(\mathrm{d}x + i\mathrm{d}y) \\
&= \oint_C (u\mathrm{d}x - v\mathrm{d}y) + i\oint_C (v\mathrm{d}x + u\mathrm{d}y) \\
&= \iint_D \left(-\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}\right)\mathrm{d}x\mathrm{d}y + i\iint_D \left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right)\mathrm{d}x\mathrm{d}y = 0
\end{aligned} \tag{230}$$

□

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

$$\int_{C_1} f(z)\mathrm{d}z = \int_{C_2} f(z)\mathrm{d}z \tag{231}$$

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

$$\oint_C f(z)\mathrm{d}z = \int_{C_1} f(z)\mathrm{d}z - \int_{C_2} f(z)\mathrm{d}z = 0 \tag{232}$$

□

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

$$\oint_{C_1} f(z)\mathrm{d}z = \oint_{C_2} f(z)\mathrm{d}z \tag{233}$$

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

$$\begin{aligned}\oint_C f(z)\mathrm{d}z &= \left(\int_{C_1} + \int_{\overline{BA}} - \int_{C_2} + \int_{\overline{AB}}\right) f(z)\mathrm{d}z \\ &= \int_{C_1} f(z)\mathrm{d}z - \int_{C_2} f(z)\mathrm{d}z = 0\end{aligned} \tag{234}$$

□

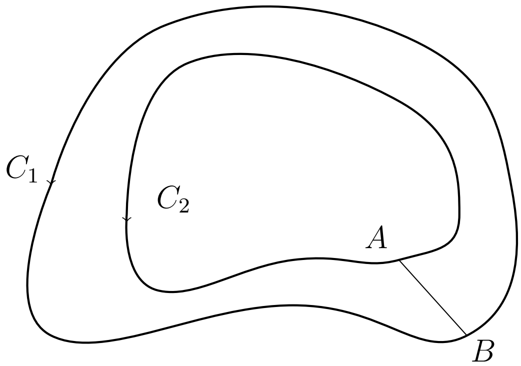

Figure 6: The constructed contour C_1 and C_2 for the proof of contour deformation.

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

$$z = \mathrm{e}^{i\theta}, \qquad \mathrm{d}z = i\mathrm{e}^{i\theta}\mathrm{d}\theta \tag{235}$$

then

$$\oint_C \frac{1}{z}\mathrm{d}z = \oint_{|z|=1} \frac{1}{z}\mathrm{d}z = \int_{-\pi}^{\pi} \mathrm{e}^{-i\theta} i\mathrm{e}^{i\theta}\mathrm{d}\theta = 2\pi i \tag{236}$$

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

$$\oint_C \frac{f(z)}{z - z_0}\mathrm{d}z = 2\pi i f(z_0) \tag{237}$$

or

$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z - z_0} \mathrm{d}z \tag{238}$$

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

$$\begin{aligned} \oint_C \frac{f(z)}{z - z_0} \mathrm{d}z &= \lim_{r \to 0} \oint_{C_r} \frac{f(z)}{z - z_0} \mathrm{d}z = \lim_{r \to 0} \int_0^{2\pi} \frac{f(z_0 + r\mathrm{e}^{i\theta})}{r\mathrm{e}^{i\theta}} ir\mathrm{e}^{i\theta} \mathrm{d}\theta \\ &= \lim_{r \to 0} i \int_0^{2\pi} f(z_0 + r\mathrm{e}^{i\theta}) \mathrm{d}\theta = 2\pi i f(z_0) \end{aligned} \tag{239}$$

□

Example. Consider the integral

$$\oint \frac{\sin z}{z^2 + 1} \mathrm{d}z = \oint_C \frac{\sin z}{(z + i)(z - i)} \mathrm{d}z \tag{240}$$

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

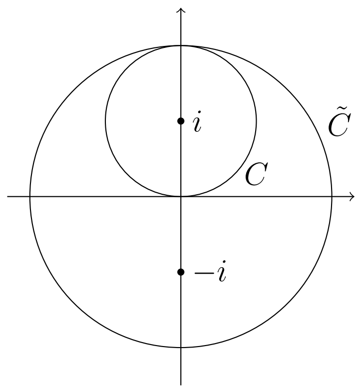

Figure 7: The contour C and $\tilde{C}$ for the example.

(1) For the contour C, We choose

$$f(z) = \frac{\sin z}{z + i} \tag{241}$$

Then

$$\oint_C \frac{\sin z}{z^2 + 1} \mathrm{d}z = \oint_C \frac{f(z)}{z - i} \mathrm{d}z = 2\pi i \frac{\sin i}{2i} = \pi i \sinh 1 \tag{242}$$

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

$$\begin{aligned} \oint_{\tilde{C}} \frac{\sin z}{z^2 + 1} \mathrm{d}z &= \oint_{\tilde{C}} \frac{\sin z}{(z + i)(z - i)} \mathrm{d}z = \frac{i}{2} \oint_{\tilde{C}} \left(\frac{\sin z}{z + i} - \frac{\sin z}{z - i} \right) \mathrm{d}z \\ &= -\pi(\sin(-i) - \sin(i)) = 2\pi i \sinh 1 \end{aligned} \tag{243}$$

5.4.6 Derivatives of Analytic Functions

Cauchy's integral theorem gives

$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z - z_0} \mathrm{d}z \tag{244}$$

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

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

Similarly,

$$f''(z_0) = \frac{2!}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^3} \mathrm{d}z \tag{246}$$

$$\vdots$$

$$f^{(n)}(z_0) = \frac{n!}{2\pi i} \oint_C \frac{f(z_0)}{(z - z_0)^{n+1}} \mathrm{d}z \tag{247}$$

Example. Consider the integral

$$I = \oint_C \frac{1}{z^n} \mathrm{d}z = \oint_C \frac{f(z)}{z^{n+1}} \mathrm{d}z \quad \text{with} \quad C : |z| = r \tag{248}$$

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

$$\int_{-\infty}^{\infty} \mathrm{e}^{-x^2} \mathrm{d}x = \int_{-\infty}^{\infty} \mathrm{e}^{-(x'+ia)^2} \mathrm{d}x' \tag{249}$$

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

$$I_1 = \int_{-\infty}^{\infty} \mathrm{e}^{-x^2} \mathrm{d}x = \int_{C_1} \mathrm{e}^{-z^2} \mathrm{d}z \tag{250}$$

$$I_2 = \int_{-\infty}^{\infty} \mathrm{e}^{-(x'+ia)^2} \mathrm{d}x' = \int_{C_2} \mathrm{e}^{-z^2} \mathrm{d}z \tag{251}$$

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

$$\oint_{C_R} \mathrm{e}^{-z^2} \mathrm{d}z = 0 \tag{252}$$

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

$$\lim_{R\to\infty} \oint_{C_R} \mathrm{e}^{-z^2} \mathrm{d}z = \lim_{R\to\infty} \left(\int_{C_1} + \int_{E_R^+} - \int_{C_2} + \int_{E_R^-} \right) \mathrm{e}^{-z^2} \mathrm{d}z = 0 \tag{253}$$

Now

$$\lim_{R\to\infty} \int_{E_R^+} \mathrm{e}^{-z^2} \mathrm{d}z = \lim_{R\to\infty} \int_0^a \mathrm{e}^{-(R+iy)^2} i\mathrm{d}y = 0 \tag{254}$$

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

So we have $I_1 = I_2$. $\square$

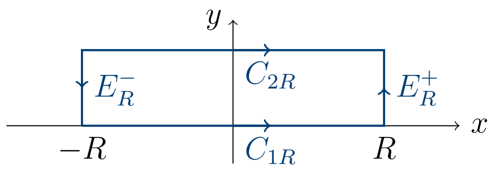

Figure 8: The contour C_R.

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

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_n)^2 \tag{256}$$

where

$$a_n = \frac{f^{(n)}(z_0)}{n!} = \frac{1}{2\pi i} \oint_C \frac{f(z)}{(z-z_0)^{n+1}} \mathrm{d}z \tag{257}$$

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.

$$f(z) = \frac{\mathrm{e}^z}{(z-5)(z+i)(z-(1+i))^2} \tag{258}$$

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.*

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

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

$$f(z) = \sum_{n=0}^{\infty} a_n (z-z_0)^n + \sum_{n=1}^{m} \frac{b_n}{(z-z_0)^n} \tag{260}$$

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

$$f(z) = \sum_{n=0}^{\infty} a_n (z-z_0)^n + \sum_{n=1}^{\infty} \frac{b_n}{(z-z_0)^n} \tag{261}$$

Example.

$$f(z) = \mathrm{e}^{1/z} = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{1}{z}\right)^n \tag{262}$$

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*

$$\mathrm{Res}_f(z_0) = \frac{1}{2\pi i} \oint_{C_{z_0}} f(z)\mathrm{d}z \tag{263}$$

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

$$f(z) = \frac{g(z)}{(z-z_0)^m} \tag{264}$$

and

$$\mathrm{Res}_f(z_0) = \frac{1}{2\pi i} \oint_C \frac{g(z)}{(z-z_0)^m}\mathrm{d}z = \frac{1}{(m-1)!} \left.\frac{\mathrm{d}^{m-1} g(z)}{\mathrm{d}z^{m-1}}\right|_{z=z_0} \tag{265}$$

Example.

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

$$\mathrm{Res}_f(z_0) = 1 \tag{266}$$

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

$$\mathrm{Res}_f(-1) = \left.\frac{\mathrm{d}\sin z}{\mathrm{d}z}\right|_{z=-1} = \cos(-1) = \cos 1 \tag{267}$$

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

$$\oint_C f(z)\mathrm{d}z = 2\pi i \sum_{k=1}^{N} \mathrm{Res}_f(z_k) \tag{268}$$

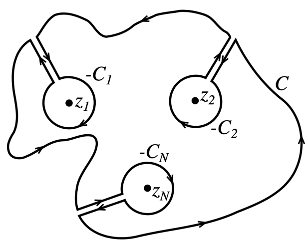

Figure 9: The contour C used in the proof of the residue theorem.

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

$$\oint_{\tilde{C}} f(z)\mathrm{d}z = \oint_C f(z)\mathrm{d}z - 2\pi i \sum_{k=1}^{N} \mathrm{Res}_f(z_k) = 0 \tag{269}$$

□

5.6.2 Contour Integration Examples

Example.

(1)

$$I = \oint_{|z|=1} \mathrm{e}^{1/z}\mathrm{d}z = \oint_{|z|=1} \left[1 + \frac{1}{z} + \frac{1}{2!}\left(\frac{1}{z}\right)^2 + \cdots\right]\mathrm{d}z = 2\pi i \tag{270}$$

(2)

$$\begin{aligned} I = &\oint_{|z|=3} \frac{z+2}{2z^2+1}\mathrm{d}z = \oint_{|z|=3} \frac{z+2}{2(z+\frac{i}{\sqrt{2}})(z-\frac{i}{\sqrt{2}})}\mathrm{d}z \\ =&2\pi i \left[\mathrm{Res}\left(\frac{i}{\sqrt{2}}\right) + \mathrm{Res}\left(-\frac{i}{\sqrt{2}}\right)\right] \\ =&2\pi i \left[\frac{\frac{i}{\sqrt{2}}+2}{2(\frac{i}{\sqrt{2}}+\frac{i}{\sqrt{2}})} + \frac{-\frac{i}{\sqrt{2}}+2}{2(-\frac{i}{\sqrt{2}}-\frac{i}{\sqrt{2}})}\right] = \pi i \end{aligned} \tag{271}$$

(3)

$$I = \int_{-\infty}^{\infty} \frac{\mathrm{d}x}{(x^2+1)(x^2+9)} \tag{272}$$

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

$$\begin{aligned}
I =& \lim_{R\to\infty} \int_{-R}^{R} \frac{\mathrm{d}x}{(x^2+1)(x^2+9)} = \lim_{R\to\infty} \int_{S_R} \frac{\mathrm{d}z}{(z^2+1)(z^2+9)} \\
=& \lim_{R\to\infty} \oint_C \frac{\mathrm{d}z}{(z+i)(z-i)(z+3i)(z-3i)} - \lim_{R\to\infty} \int_{C_R} \frac{\mathrm{d}z}{(z^2+1)(z^2+9)} \\
=& 2\pi i \left[\mathrm{Res}(i) + \mathrm{Res}(3i)\right] - \lim_{R\to\infty} \frac{iR}{(R^2+1)(R^2+9)} \int_0^{\pi} \mathrm{e}^{i\theta} \mathrm{d}\theta \\
=& 2\pi i \left(\frac{1}{16i} + \frac{1}{-48i} \right) = \frac{\pi}{12}
\end{aligned} \tag{273}$$

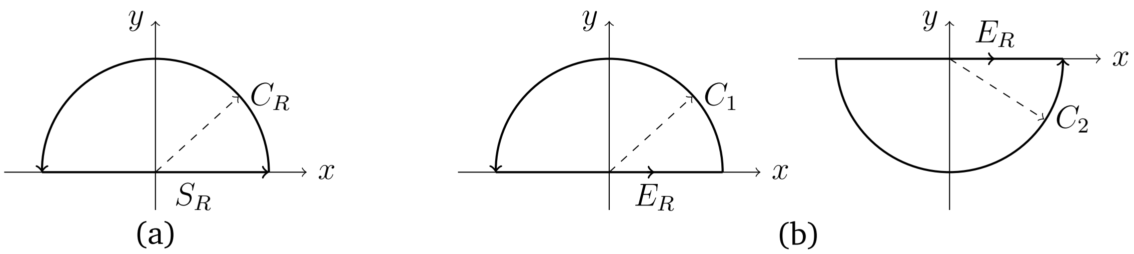

Figure 10: (a) The contour for example (3). (b) The contour for example (4).

(4)

$$\begin{aligned}
I =& \int_{-\infty}^{\infty} \frac{\cos x}{x^2+1} \mathrm{d}x = \int_{x-\mathrm{axis}} \frac{\cos z}{z^2+1} \mathrm{d}z \\
=& \int_{x-\mathrm{axis}} \frac{\mathrm{e}^{iz}}{2(z+i)(z-i)} \mathrm{d}z + \int_{x-\mathrm{axis}} \frac{\mathrm{e}^{-iz}}{2(z+i)(z-i)} \mathrm{d}z \\
=& I_1 + I_2
\end{aligned} \tag{274}$$

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

$$\begin{aligned}
I_1 =& \lim_{R\to\infty} \oint_{\tilde{C}_1} \frac{\mathrm{e}^{iz}}{2(z+i)(z-i)} \mathrm{d}z - \lim_{R\to\infty} \int_{C_1} \frac{\mathrm{e}^{iz}}{2(z+i)(z-i)} \mathrm{d}z \\
=& 2\pi i\, \mathrm{Res}(i) - \lim_{R\to\infty} \int_0^{\pi} \frac{\mathrm{e}^{iR\mathrm{e}^{i\theta}}}{2(R^2+1)} iR\mathrm{e}^{i\theta} \mathrm{d}\theta = 2\pi i \frac{\mathrm{e}^{-1}}{4i} - 0 = \frac{\pi}{2}\mathrm{e}^{-1}
\end{aligned} \tag{275}$$

$$\begin{aligned}
I_2 =& - \lim_{R\to\infty} \oint_{\tilde{C}_2} \frac{\mathrm{e}^{-iz}}{2(z+i)(z-i)} \mathrm{d}z + \lim_{R\to\infty} \int_{C_2} \frac{\mathrm{e}^{-iz}}{2(z^2+1)} \mathrm{d}z \\
=& - 2\pi i\, \mathrm{Res}(-i) + \lim_{R\to\infty} \int_{-\pi}^{0} \frac{\mathrm{e}^{-iR\mathrm{e}^{i\theta}}}{2(R^2+1)} iR\mathrm{e}^{i\theta} \mathrm{d}\theta \\
=& - 2\pi i \frac{\mathrm{e}^{-1}}{-4i} + 0 = \frac{\pi}{2}\mathrm{e}^{-1}
\end{aligned} \tag{276}$$

So we have

$$I = I_1 + I_2 = \pi \mathrm{e}^{-1} \tag{277}$$

5.6.3 Jordan's Lemma

Lemma. Consider

$$I(R) = \int_{C_R} \mathrm{e}^{i\alpha z} f(z)\mathrm{d}z \tag{278}$$

where $\alpha > 0$ ($\alpha < 0$) and C_R is a semicircle of radius R in the upper (lower) half-plane. Let $M(R)$ be the maximum value of $f(z)$ on C_R. If $M(R) \to 0$ as $R \to \infty$, so dose $I(R)$.

Proof. Consider the case $\alpha > 0$ and C_R is a semicircle of radius R in the upper half-plane.

$$|I(R)| = \left| \int_{C_R} \mathrm{e}^{i\alpha z} f(z)\mathrm{d}z \right| \le \int_{C_R} |\mathrm{e}^{i\alpha z}||f(z)||\mathrm{d}z| \tag{279}$$

At the point $z = R\mathrm{e}^{i\theta}$ on the contour, we have

$$\begin{cases} |\mathrm{e}^{i\alpha z}| = \mathrm{e}^{-\alpha y} = \mathrm{e}^{-\alpha R \sin\theta} \\ |f(z)| \le M(R) \\ |\mathrm{d}z| = R\mathrm{d}\theta \end{cases} \tag{280}$$

so

$$\begin{aligned} |I(R)| &\le M(R) \int_0^{\pi} \mathrm{e}^{-\alpha R \sin\theta} R\mathrm{d}\theta = 2RM(R) \int_0^{\pi/2} \mathrm{e}^{-\alpha R \sin\theta} \mathrm{d}\theta \\ &\le 2RM(R) \int_0^{\pi/2} \mathrm{e}^{-\alpha R(2\theta/\pi)} \mathrm{d}\theta = \frac{\pi M(R)}{\alpha}(1 - \mathrm{e}^{-\alpha R}) \le \frac{\pi M(R)}{\alpha} \end{aligned} \tag{281}$$

Thus, if $M(R) \to 0$ as $R \to \infty$, so dose $I(R)$. □

5.6.4 Inverse Laplace Transforms

Suppose we know

$$F(s) = \mathcal{L}[f(t)] = \int_0^{s} f(t)\mathrm{e}^{-st}\mathrm{d}t \tag{282}$$

and we want to find

$$f(t) = \mathcal{L}^{-1}[F(s)] = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} F(s)\mathrm{e}^{st}\mathrm{d}s \tag{283}$$

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

$$f(t) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} F(s)\mathrm{e}^{st}\mathrm{d}s = \sum_i \mathrm{Res}(a_i) - \lim_{R\to\infty}\int_{C_R} F(s)\mathrm{e}^{st}\mathrm{d}s \tag{284}$$

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

$$f(t) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} F(s)\mathrm{e}^{st}\mathrm{d}s = \sum_i \mathrm{Res}(a_i), \qquad t > 0 \tag{285}$$

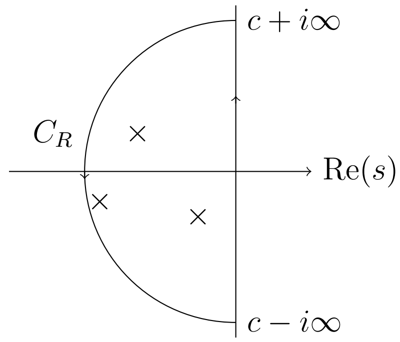

Figure 11: The contour for inverting Laplace transforms.

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 $f(x)$

$$f(x+\delta x) = f(x) + \delta x f'(x) + \frac{(\delta x)^2}{2}f''(x) + \cdots \tag{286}$$

At a stationary point $x = x_0$

$$f'(x_0) = 0 \tag{287}$$

$$\delta f(x) = f(x+\delta x) - f(x) = \mathcal{O}(\delta x^2) \tag{288}$$

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

$$\delta I = I[y+\delta y] - I[y] \tag{289}$$

Seek $y = y_0$ such that

$$\delta I|_{y_0} = \mathcal{O}(\delta y^2) \tag{290}$$

6.2 Euler-Lagrange Problem

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

$$I[y] = \int_{x_A}^{x_B} f(x, y(x), y'(x))\mathrm{d}x \tag{291}$$

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

$$y(x) \to y(x) + \delta y(x) \tag{292}$$

then

$$\begin{aligned} I[y+\delta y] &= \int_{x_A}^{x_B} f(x, y(x) + \delta y(x), y' + \delta y'(x)) \mathrm{d}x \\ &= \int_{x_A}^{x_B} \left[f(x,y,y') + \delta y \frac{\partial f}{\partial y} + \delta y' \frac{\partial f}{\partial y'} + \mathcal{O}(\delta y^2) \right] \mathrm{d}x \end{aligned} \tag{293}$$

so we have

$$\begin{aligned} \delta I =& I[y+\delta y] - I[y] \\ =& \int_{x_A}^{x_B} \left(\delta y \frac{\partial f}{\partial y} + \delta y' \frac{\partial f}{\partial y'} \right) \mathrm{d}x + \mathcal{O}(\delta y^2) \\ =& \int_{x_A}^{x_B} \left(\delta y \frac{\partial f}{\partial y} \right) \mathrm{d}x + \left[\delta y \frac{\partial f}{\partial y'} \right]_{x_A}^{x_B} - \int_{x_A}^{x_B} \delta y \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\partial f}{\partial y'} \right) \mathrm{d}x + \mathcal{O}(\delta y^2) \\ =& \int_{x_A}^{x_B} \delta y \left[\frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\partial f}{\partial y'} \right) \right] \mathrm{d}x + \mathcal{O}(\delta y^2) \end{aligned} \tag{294}$$

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

$$\boxed{\frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\partial f}{\partial y'} \right) = 0} \tag{295}$$

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

Example.

$$f(x,y,y') = (1+x^2) y'^2 - y^4 \tag{296}$$

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

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

We can also use the original method of calculus of variations

$$I[y+\delta y] = \int_{x_A}^{x_B} \left[(1+x^2)(y' + \delta y')^2 - (y+\delta y)^4 \right] \mathrm{d}x \tag{298}$$

so

$$\begin{aligned} \delta I =& \int_{x_A}^{x_B} \left[(1+x^2) 2y' \delta y' - 4y^3 \delta y \right] \mathrm{d}x \\ =& (1+x^2) 2y' \delta y \Big|_{x_A}^{x_B} - \int_{x_A}^{x_B} \mathrm{d}x \left(\delta y \frac{\mathrm{d}}{\mathrm{d}x} [(1+x^2) 2y'] + 4y^3 \delta y \right) \mathrm{d}x \\ =& \int_{x_A}^{x_B} \mathrm{d}x \delta y \left(-\frac{\mathrm{d}}{\mathrm{d}x} [(1+x^2) 2y'] - 4y^3 \right) \mathrm{d}x \end{aligned} \tag{299}$$

I is stationary if

$$-\frac{\mathrm{d}}{\mathrm{d}x}[(1+x^2)2y'] - 4y^3 = 0 \tag{300}$$

6.2.1 Beltrami identity

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

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}x} + \frac{\partial f}{\partial y'}\frac{\mathrm{d}y'}{\mathrm{d}x} \tag{301}$$

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

$$\begin{aligned}\frac{\mathrm{d}f}{\mathrm{d}x} =& \frac{\partial f}{\partial x} + y'\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'}\right) + y''\frac{\partial f}{\partial y'} \\ =& \frac{\partial f}{\partial x} + \frac{\mathrm{d}}{\mathrm{d}x}\left(y'\frac{\partial f}{\partial y'}\right)\end{aligned} \tag{302}$$

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

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(f - \frac{\partial f}{\partial y'}y'\right) = 0 \tag{303}$$

which integrates to

$$\boxed{f - \frac{\partial f}{\partial y'}y' = \text{const}} \tag{304}$$

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

Example.

$$I[y] = \int f\mathrm{d}x \quad \text{with} \quad f(y, y') = y'^2 - y^4 \tag{305}$$

Applying the Beltrami identity

$$y'^2 - y^4 - 2y'^2 = \text{const} \tag{306}$$

6.2.2 Functional Derivatives

We know that

$$\delta I = \int_{x_A}^{x_B} \delta y \left[\frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'}\right)\right] \mathrm{d}x + \mathcal{O}(\delta y^2) \tag{307}$$

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

$$\frac{\delta I}{\delta y(x)} = \frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'}\right) \tag{308}$$

then Euler-Lagrange equation can be written as[3]

$$\frac{\delta I}{\delta y(x)} = 0 \tag{309}$$

[3] 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

$$L = T - V = \frac{1}{2}m\dot{\boldsymbol{x}}^2 + V(\boldsymbol{x}, t) \tag{310}$$

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

$$S[\boldsymbol{x}(t)] = \int_{t_A}^{t_B} L(t, \boldsymbol{x}, \dot{\boldsymbol{x}})\mathrm{d}t \tag{311}$$

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

$$\frac{\partial L}{\partial x_i} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}_i}\right) = 0, \qquad i = 1, 2, 3 \tag{312}$$

these give

$$m\ddot{x}_i = -\nabla_i V, \qquad i = 1, 2, 3 \tag{313}$$

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

$$\mathrm{d}s = \sqrt{\mathrm{d}x^2 + \mathrm{d}y^2} = \sqrt{1 + \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2}\mathrm{d}x \tag{314}$$

so the length of $y(x)$ is

$$\int \mathrm{d}s = \int_{x_A}^{x_B} \sqrt{1 + y'^2}\mathrm{d}x \tag{315}$$

This extremised by Euler-Lagrange equation

$$0 - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{y'}{\sqrt{1 + y'^2}}\right) = 0 \quad \Rightarrow \quad y' = c \quad \Rightarrow \quad y = cx + d \tag{316}$$

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

$$y = y(\lambda), \qquad x = x(\lambda) \tag{317}$$

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

$$\int \mathrm{d}s = \int \sqrt{\mathrm{d}x^2 + \mathrm{d}y^2} = \int_{\lambda_A}^{\lambda_B} \sqrt{\left(\frac{\mathrm{d}x}{\mathrm{d}\lambda}\right)^2 + \left(\frac{\mathrm{d}y}{\mathrm{d}\lambda}\right)^2}\mathrm{d}\lambda \tag{318}$$

This extremised by Euler-Lagrange equation. For x

$$0 - \frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\frac{x'}{\sqrt{x'^2 + y'^2}}\right) = 0 \quad \Rightarrow \quad \frac{x'}{\sqrt{x'^2 + y'^2}} = \alpha \tag{319}$$

Similarly, for y

$$0 - \frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\frac{y'}{\sqrt{x'^2 + y'^2}}\right) = 0 \quad \Rightarrow \quad \frac{y'}{\sqrt{x'^2 + y'^2}} = \beta \tag{320}$$

So we have

$$\frac{y'}{x'} = \gamma \quad \Rightarrow \quad \frac{\mathrm{d}y}{\mathrm{d}x} = \gamma \quad \Rightarrow \quad y = \gamma x + c \tag{321}$$

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

$$T = \int_A^B \mathrm{d}t = \int_A^B \frac{\mathrm{d}s}{v} = \int_{x=0}^{x=x_B} \frac{\sqrt{1+y'^2}}{\sqrt{2gy}}\mathrm{d}x \tag{322}$$

Using the Beltrami identity

$$\frac{\sqrt{1+y'^2}}{\sqrt{2gy}} - \frac{\frac{y'}{\sqrt{1+y'^2}}}{\sqrt{2gy}}y' = c \quad \Rightarrow \quad y(1+y'^2) = c^2 \quad \Rightarrow \quad y' = \sqrt{\frac{\alpha - y}{y}} \tag{323}$$

where $\alpha = c^2$. The solution is a cycloid[4]

$$x = x(\theta) = a(\theta - \sin\theta) \tag{324}$$

$$y = y(\theta) = a(1 - \cos\theta) \tag{325}$$

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

$$T = \int_0^{\theta_B} \frac{\sqrt{(\mathrm{d}x/\mathrm{d}\theta)^2 + (\mathrm{d}y/\mathrm{d}\theta)^2}}{\sqrt{2gy}}\mathrm{d}\theta = \int_0^{\theta_B} \sqrt{\frac{a}{g}}\mathrm{d}\theta = \sqrt{\frac{a}{g}}\theta_B \tag{326}$$

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

$$L(x, \dot{x}) = T - L = \frac{1}{2}m\dot{x}^2 - V(x) \tag{327}$$

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

Using the Beltrami identity

$$L - \frac{\partial L}{\partial \dot{x}}\dot{x} = \text{const} \tag{328}$$

which gives

$$\frac{1}{2}m\dot{x}^2 + V = \underbrace{T + V}_{\text{total energy}} = \text{const} \tag{329}$$

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 $\boldsymbol{q}$

$$L(\boldsymbol{q}, \dot{\boldsymbol{q}}) = T - V(\boldsymbol{q}), \qquad \boldsymbol{q} = (q_1, q_2, \cdots, q_N) \tag{330}$$

which does not depend on t. If one defines

$$H = -L + \sum_{i=1}^{N} \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} \tag{331}$$

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

$$\frac{\partial V}{\partial x_i} = 0, \qquad i = 1, 2, 3 \tag{332}$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}_i}\right) = 0 \quad \Rightarrow \quad m\dot{x}_i = \text{const} \tag{333}$$

  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

$$L = T - V(r, \theta, \phi) \tag{334}$$

  where the kinetic energy

$$T = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\dot{\phi}^2) \tag{335}$$

  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.

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{\phi}}\right) = \frac{\partial L}{\partial \phi} = 0 \quad \Rightarrow \quad mr^2\sin^2\theta\dot{\phi} = \text{const} \tag{336}$$

  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

$$g(x, y) - C = 0 \tag{337}$$

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

$$\nabla f(P) \parallel \nabla g(P) \quad \Rightarrow \quad \nabla \left(f(x, y) - \lambda g(x, y)\right)_P = 0 \tag{338}$$

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

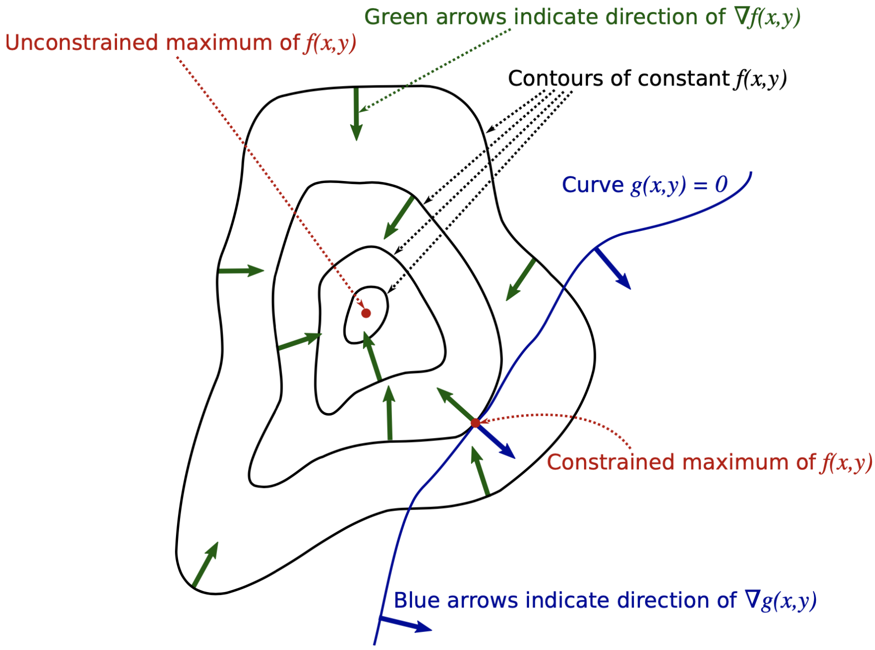

Figure 12: An illustration of the method of Lagrange multipliers.

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

$$\begin{aligned} g_1(\boldsymbol{x}) &= C_1 \\ g_2(\boldsymbol{x}) &= C_2 \\ &\vdots \\ g_k(\boldsymbol{x}) &= C_k \end{aligned} \tag{339}$$

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

$$\nabla(f - \lambda_1 g_1 - \lambda_2 g_2 - \cdots - \lambda_k g_k) = 0 \tag{340}$$

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

$$f(x_1, x_2, y_1, y_2) = (x_2 - x_1)^2 + (y_2 - y_1)^2 \tag{341}$$

Construct

$$u(x_1, x_2, y_1, y_2) = f(x_1, x_2, y_1, y_2) + \lambda_1 x_1 y_1 + \mu(x_2 + 2y_2) \tag{342}$$

$\boldsymbol{\nabla} u = 0$ gives

$$\frac{\partial u}{\partial x_1} = 2(x_1 - x_2) + \lambda_1 y_1 = 0 \tag{343}$$

$$\frac{\partial u}{\partial x_2} = 2(x_2 - x_1) + \mu_2 = 0 \tag{344}$$

$$\frac{\partial u}{\partial y_1} = 2(y_1 - y_2) + \lambda_1 x_1 = 0 \tag{345}$$

$$\frac{\partial u}{\partial y_2} = 2(y_2 - y_1) + 2\mu_2 = 0 \tag{346}$$

The solution is

$$(x_1, y_1) = \left(\sqrt{2}, \frac{\sqrt{2}}{2}\right), \qquad (x_2, y_2) = \left(\frac{1 + 3\sqrt{2}}{5}, \frac{4 - 3\sqrt{2}}{10}\right) \tag{347}$$

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

$$E = g \int_A^B y \mathrm{d}m = \rho g \int_A^B y \mathrm{d}s = \rho g \int_{-a}^{a} y \sqrt{1 + \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2} \mathrm{d}x \tag{348}$$

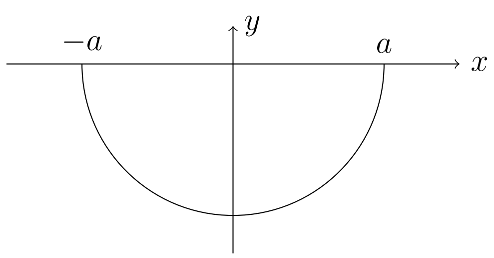

Figure 13: A heavy rope of a chain hanging between two fixed end points $A(-a, 0)$ and $B(a, 0)$.

The length of the rope is fixed. So the constraint

$$L = \int_A^B \mathrm{d}s = \int_{-a}^{a} \sqrt{1 + \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2} \mathrm{d}x \tag{349}$$

Then we have to extremise

$$\begin{aligned} U = E - \lambda L =& \rho g \int_{-a}^{a} y \sqrt{1 + \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2} \mathrm{d}x - \lambda \int_{-a}^{a} \sqrt{1 + \left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)^2} \mathrm{d}x \\ =& \int_{-a}^{a} (\rho g y - \lambda) \sqrt{1 + y'^2} \mathrm{d}x = \int_{-a}^{a} f \mathrm{d}x \end{aligned} \tag{350}$$

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

$$f - \frac{\partial f}{\partial y'} y' = C \tag{351}$$

which is

$$(\rho g y - \lambda)\sqrt{1 + y'^2} - (\rho g y - \lambda)\frac{y'^2}{\sqrt{1 + y'^2}} = C \tag{352}$$

$$\rho g y - \lambda = C\sqrt{1 + y'^2} \tag{353}$$

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

$$\eta = C\sqrt{1 + \frac{\eta'^2}{\rho^2 g^2}}, \qquad \eta' = \pm \rho g \sqrt{\frac{\eta^2}{C^2} - 1} \tag{354}$$

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

$$\eta' = \frac{\mathrm{d}\eta}{\mathrm{d}x} = \rho g \sqrt{\frac{\eta^2}{C^2} - 1} \quad \Rightarrow \quad \frac{\mathrm{d}\eta}{\sqrt{\frac{\eta^2}{C^2} - 1}} = \rho g \mathrm{d}x \tag{355}$$

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

$$\begin{aligned} \int \frac{\mathrm{d}\eta}{\sqrt{\frac{\eta^2}{C^2} - 1}} &= \rho g \int \mathrm{d}x \\ \Rightarrow \quad C \int \mathrm{d}q &= \rho g \mathrm{d}x \\ \Rightarrow \quad Cq &= \rho g x + d \\ \Rightarrow \quad \frac{\eta}{C} &= \cosh\left(\frac{\rho g x + d}{C}\right) \end{aligned} \tag{356}$$

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

$$y(x) = \frac{1}{\rho g}\left[\cosh\left(\frac{\rho g x}{C}\right) + \lambda\right] \tag{357}$$

The two constraints

1. When $x = a$, $y = 0$
$$\frac{1}{\rho g}\left[\cosh\left(\frac{\rho g a}{C} + \lambda\right)\right] = 0 \tag{358}$$

2. The length of the rope is fixed
$$L = \int_{-a}^{a} \cosh\left(\frac{\rho g x}{C}\right) \mathrm{d}x = \frac{C}{\rho g}\sinh\frac{\rho g x}{C}\bigg|_{-a}^{a} = \frac{2C}{\rho g}\sinh\frac{\rho g a}{C} \tag{359}$$

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

$$E[\psi] = \int \psi^* \hat{H}\psi \tag{360}$$

subject to the normalisation constraint

$$\int \psi^*\psi = 1 \tag{361}$$

We claim that
$$I[\psi] = \int \psi^*\hat{H}\psi - \varepsilon \int \psi^*\psi \tag{362}$$

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

$$\begin{aligned}\delta I =& I[\psi + \delta\psi] - I[\psi] \\ =& \int (\delta\psi^*)\hat{H}\psi + \int \psi^*\hat{H}(\delta\psi) - \varepsilon\int(\delta\psi^*)\psi - \varepsilon\int\psi^*(\delta\psi) \\ =& \int(\delta\psi^*)(\hat{H}\psi - \varepsilon\psi) + \int(\delta\psi)(\hat{H}\psi - \varepsilon\psi)^* = 0\end{aligned} \tag{363}$$

$$\begin{aligned}\delta I =& I[\psi + i\delta\psi] - I[\psi] \\ =& -i\int (\delta\psi^*)\hat{H}\psi + i\int \psi^*\hat{H}(\delta\psi) + i\varepsilon\int(\delta\psi^*)\psi - i\varepsilon\int\psi^*(\delta\psi) \\ =& -i\int(\delta\psi^*)(\hat{H}\psi - \varepsilon\psi) + i\int(\delta\psi)(\hat{H}\psi - \varepsilon\psi)^* = 0\end{aligned} \tag{364}$$

Compare the two equations, we have

$$\int(\delta\psi^*)(\hat{H}\psi - \varepsilon\psi) = 0 \tag{365}$$

for any ψ. Hence
$$\hat{H}\psi - \varepsilon\psi = 0 \tag{366}$$

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

$$\tilde{\psi}(\boldsymbol{c}) = \sum_{\alpha=1}^{M} c_\alpha \phi_\alpha \tag{367}$$

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

$$I[\tilde{\psi}] = I[\boldsymbol{c}] = E[\boldsymbol{c}] - \varepsilon N[\boldsymbol{c}] \tag{368}$$

Here, E is the total energy of the system

$$E[\boldsymbol{c}] = \int \sum_{\alpha=1}^{M} c_\alpha^* \phi_\alpha^* \hat{H} \sum_{\beta=1}^{M} c_\beta \phi_\beta = \sum_{\alpha,\beta=1}^{M} c_\alpha^* H_{\alpha\beta} c_\beta \tag{369}$$

and N is the normalisation constraint.

$$N[\boldsymbol{c}] = \int \sum_{\alpha}^{M} c_\alpha^* \phi_\alpha^* \sum_{\beta}^{M} c_\beta \phi_\beta = \int \sum_{\alpha,\beta=1}^{M} c_\alpha^* S_{\alpha\beta} c_\beta \tag{370}$$

where

$$H_{\alpha\beta} = \int \phi_\alpha^* \hat{H} \phi_\beta = \text{Hamiltonian matrix} \tag{371}$$

$$S_{\alpha\beta} = \int \phi_\alpha^* \phi_\beta = \text{overlap matrix} \tag{372}$$

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