# Eigenphysics II

# Contents

# List of Figures

# Chapter 1

# Function Spaces: Infinite-Dimensional Vector Spaces

## 1.1 Linear Independence of Monomials

A critical fact is that, on any interval, the functions $1, x, x^2, \ldots, x^n$ are linearly independent.

To do this we introduce $n$ copies of these functions, this may seem like over-kill, but we will see that it leads to a straightforward proof of the claim. But first let us make some preliminary comments. If an $n-th$ order polynomial $p(x) = a_n x^n + \cdots + a_2 x^2 + a_1 x + a_0$ has the $n$ roots $\alpha_1, \alpha_2, \ldots, \alpha_n$ then we can write

$$p(x) = p(x) - p(\alpha_1) = a_n(x^n - \alpha_1^n) + \cdots + a_2(x^2 - \alpha_1^2)x^2 + a_1(x - \alpha_1).$$

Using

$$x^r - \alpha_1^r = (x - \alpha_1)(x^{r-1} + x^{r-2}\alpha_1 + \cdots + \alpha_1^{r-1})$$

we have

$$\begin{aligned} p(x) &= p(x) - p(\alpha_1) \\ &= a_n(x - \alpha_1)(x^{n-1} + a_1^{n-2}\alpha_1 + \ldots x^{n-1}) + \cdots + a_2(x - \alpha_1)(x + \alpha_1) + a_1(x - \alpha_1) \\ &= (x - \alpha_1)[a_n(x^{r-1} + x^{r-2}\alpha_1 + \ldots \alpha_1^{r-1}) + \cdots + a_2(x - \alpha_1) + a_1] \end{aligned} \tag{1.1}$$

what is in the square brackets is an $(n-1)-th$ order polynomial in $x$. We can apply the same argument to this. Continuing in this way we obtain

$$p(x) = a_n(x-\alpha_1)(x-\alpha_2)\dots(x-\alpha_n)$$

Now we move onto the proof of the main result. The linear independence is controlled by the following determinant

$$\Delta_n = \det \mathbf{M}_n = \det \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ x_1 & x_2 & x_3 & \cdots & x_n \\ x_1^2 & x_2^2 & x_3^2 & \cdots & x_n^2 \\ x_1^3 & x_2^3 & x_3^3 & \cdots & x_n^3 \\ . & . & . & \cdots & . \\ . & . & . & \cdots & . \\ x_1^{n-1} & x_2^{n-1} & x_3^{n-1} & \cdots & x_n^{n-1} \end{bmatrix} \tag{1.2}$$

Let us consider this to be a polynomial in $x_n$ with $x_1, x_2, \dots, x_{n-1}$, for the moment, treated as constants. We then have an $(n-1)-th$ order polynomial in $x_n$ and so has $n-1$ roots. The fact that the determinant vanishes when any two columns are equal it follows that $x_1, x_2, \dots, x_{n-1}$ are the roots of this polynomial and implies

$$\Delta_n = (x_n - x_1)(x_n - x_2)\dots(x_n - x_{n-1})\ q_{n-1}(x_1, x_2, \dots, x_{n-1}). \tag{1.3}$$

We then consider $q_{n-1}(x_1, x_2, \dots, x_{n-1})$ as an $(n-2)-th$ polynomial in $x_{n-1}$. This has the $n-2$ roots $x_1, x_2, \dots, x_{n-2}$ again following from the fact that the determinant vanishes when any two columns are equal (note that $x_n$ cannot be a root of $q_{n-1}(x_1, x_2, \dots, x_{n-1})$ as that would make $\Delta_n$ an $n+1-$th order polynomial in $x_n$). So that

$$\begin{aligned} \Delta_n &= [(x_n - x_1)(x_n - x_2)\dots(x_n - x_{n-1}]) \times \\ &\times[(x_{n-1} - x_1)(x_{n-1} - x_2)\dots(x_{n-1} - x_{n-2})] \times q_{n-2}(x_1, x_2, \dots, x_{n-2}) \end{aligned} \tag{1.4}$$

Continuing in this way we obtain

$$\Delta_n = \det \mathbf{M}_n = \det \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ x_1 & x_2 & x_3 & \cdots & x_n \\ x_1^2 & x_2^2 & x_3^2 & \cdots & x_n^2 \\ x_1^3 & x_2^3 & x_3^3 & \cdots & x_n^3 \\ . & . & . & \cdots & . \\ . & . & . & \cdots & . \\ x_1^{n-1} & x_2^{n-1} & x_3^{n-1} & \cdots & x_n^{n-1} \end{bmatrix} = K \prod_{i>j}(x_i - x_j) \tag{1.5}$$

It is easy to see that $\Delta_n$ is a polynomial of degree $n(n-1)/2$, and as the product $\prod_{i>j}(x_i - x_j)$ has the same degree means that $\Delta_n = K \prod_{i>j}(x_i - x_j)$ where $K$ is a constant. We can determine $K$ in the following way: First, note the in the expansion of the determinant we have the term $x_2 x_3^2 \cdots x_n^{n-1}$ with coefficient 1. Second, from the product

$$\begin{aligned} K\prod_{i>j}(x_i - x_j) &= K(x_2 - x_1)\times \\ & \quad (x_3 - x_1)(x_3 - x_2)\times \\ & \quad \vdots \\ & \quad (x_n - x_1)(x_n - x_2)\ldots(x_n - x_{n-1}) \end{aligned} \tag{1.6}$$

it is easy to see we have the term $Kx_2 x_3^2 \cdots x_n^{n-1}$. Thus $K = 1$.

We now return back to the question of linear independence of the functions $1, x, x^2 \ldots, x^n$. To say that the functions are linearly independent is equivalent to saying that

$$\lambda_1 + \lambda_2 x + \lambda_3 x^2 + \cdots + \lambda_n x^{n-1} = 0 \tag{1.7}$$

implies $\lambda_i = 0$ for $i = 1, 2, \ldots, n$. If we pick $n$ distinct points, $x_1, x_2, \ldots, x_n$, then have $n$ simultaneous linear equations for the $\lambda$'s:

$$\lambda_1 + \lambda_2 x_i + \lambda_3 x_i^2 + \cdots + \lambda_n x_i^{n-1} = 0 \tag{1.8}$$

for $i = 1, 2, \ldots, n$ which can be written in matrix form as

$$\mathbf{M}_n^T\vec{\lambda} = \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{n-1} \\ 1 & x_3 & x_3^2 & \cdots & x_3^{n-1} \\ \vdots & & \vdots & \cdots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^{n-1} \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \vdots \\ \lambda_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{1.9}$$

Recall the fact that $\hat{M}_n^T$ has an inverse if and only if its determinant, $\Delta_n$, is non-zero. Now if $\hat{M}_n^T$ has an inverse, we can multiply both sides of (1.9) on the left by the inverse of $\hat{M}_n^T$ and conclude that $\vec{\lambda} = 0$. Since the variables $x_1, x_2, \ldots, x_n$ were chosen to be distinct, the determinant, $\Delta_n$, does not vanish, and hence it follows that the functions are linearly independent.

## 1.2 Why Quantum Mechanics cant Work in Finite Dimensional Hilbert Space

Quantum mechanics for cannot work in finite-diemnsional vector spaces. We need Hermitian linear operators, $\hat{x}$ and $\hat{p}$, which satisfy,

$$[\hat{x}, \hat{p}] \equiv \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar.$$

In a finite-dimensional vector space, we can diagonalise $\hat{x}$, so that $\hat{x}|i >= x_i|i >$ and then:

$$i\hbar = i\hbar < i|i >=< i|[\hat{x}\hat{p} - \hat{p}\hat{x}]|i >= x_i < i|\hat{p}|i > -x_i < i|\hat{p}|i >= 0$$

which is contradictory. In practice we use $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ in a function space.

The 'rules' in function spaces are obviouslya bit different to those in finite vector spaces. We will proceed by doing equivalent things in function spaces unless it is seen to fail.

# Chapter 2

# Inner Products

An inner product in a function space is usually an integral over a chosen interval, with a weight:

$$(\psi_1, \psi_2) = \int_a^b dx w(x) \psi_1^*(x) \psi_2(x) \tag{2.1}$$

for $x \in (a, b)$, where $w(x)$ is a weight function,e.g. $w(x) = e^{-x}$ for $x \in (0, \infty)$, or $w(x) = e^{-x^2}$ for $x \in (-\infty, \infty)$, or $w(x) = 1$ for $x \in (-1, 1)$.

We check this has the correct properties for an inner product:

1. Linearity.

$$\begin{aligned}
(\psi, \phi_1 + \phi_2) &= \int_a^b dx w(x) \psi^*(x)[\phi_1(x) + \phi_2(x)] \\
&= \int_a^b dx w(x) \psi^*(x) \phi_1(x) + \int_a^b dx w(x) \psi^*(x) \phi_2(x) \\
&= (\psi, \phi_1) + (\psi, \phi_2)
\end{aligned}$$

2. Similar.

3. Scalar linearity.

$$\begin{aligned}
(\psi, \lambda\phi) &= \int_a^b dx w(x) \psi^*(x) \lambda \phi(x) \\
&= \lambda \int_a^b dx w(x) \psi^*(x) \phi(x) \\
&= \lambda(\psi, \phi)
\end{aligned}$$

4. Reality.

$$
\begin{aligned}
(\psi,\phi)^* &= \int_a^b dx w^*(x)\psi(x)\phi^*(x) \\
&= \int_a^b dx w(x)\phi^*(x)\psi(x) \\
&= (\phi,\psi)
\end{aligned}
$$

where we used the weight function is real valued.

5. Positivity of the norm.

$$
\begin{aligned}
(\psi,\psi) &= \int_a^b dx w^*(x)\psi^*(x)\psi(x) \\
&= \int_a^b dx w(x)|\psi(x)|^2 \\
&=
\end{aligned}
$$

is positive if $w(x)$ is positive.

## 2.1 For Quantum Mechanics

For quantum mechanics, at the outset, $w(x) = 1$ and

$$
(\psi_1,\psi_2) = \int_a^b dx \psi_1^*(x)\psi_2(x) \tag{2.2}
$$

is the inner product, with the associated norm being related to the probability of finding the particle in a certain interval.

# Chapter 3

# Integration by Parts

## 3.1 Integration by Parts

Since multiple integration by parts is the technique of the next section, we provide a quick reminder. The result derives from differentiation of a product,

$$\frac{d}{dx}(uv) = \frac{du}{dx}v + u\frac{dv}{dx}$$

and then integrating,

$$\int_a^b dx \frac{du}{dx}v = [uv]_a^b - \int_a^b dx u \frac{dv}{dx}. \tag{3.1}$$

In this form we would need to recognise the differential $\frac{du}{dx}$, but if we set $w = \frac{du}{dx}$ then,

$$\int_a^b dx w v = \left[ v(x) \int^x dx' w(x') \right]_a^b - \int_a^b dx \frac{dv}{dx}(x) \int^x dx' w(x') \tag{3.2}$$

which is how the result is usually employed.

The constant term when integrating by parts can be crucial:

## 3.2 Example 1

$$\int_0^1 dx \ln\frac{1}{1-x} = \int_0^1 dx(-1)\ln(1-x)$$
$$= [(1-x)\ln(1-x)]_0^1 - \int_0^1 dx(1-x)\frac{(-1)}{1-x} = 1 \qquad (3.3)$$

where we chose the constant to eliminate the divergence as $x \to 1$. It tends to zero by L'hopital

$$\lim_{x\to 1}(1-x)\ln(1-x) = \lim_{x\to 1}\frac{\ln(1-x)}{\frac{1}{1-x}} = \lim_{x\to 1}\frac{\frac{-1}{1-x}}{\frac{1}{(1-x)^2}} = \lim_{x\to 1}(x-1) = 0.$$

## 3.3 Example 2

We evaluate

$$I_n = \int_0^\infty dx x^n e^{-x}. \qquad (3.4)$$

Integrating by parts with $u = (-1)e^{-x}$ and $v = x^n$,

$$I_n = [(-1)e^{-x}x^n]_0^\infty + n\int_0^\infty dx x^{n-1}e^{-x} = nI_{n-1} \qquad n > 0. \qquad (3.5)$$

Now $I_0 = 1$ so:

$$I_n = n!. \qquad (3.6)$$

## 3.4 Example 3

We evaluate

$$J_n = \int_{-\infty}^\infty dx x^{2n} e^{-x^2}. \qquad (3.7)$$

Integrating by parts with $\frac{du}{dx} = xe^{-x^2}$, $u = \frac{(-1)}{2}e^{-x^2}$ and $v = x^{2n-1}$

$$\begin{aligned}
J_n &= \left[\frac{(-1)}{2}e^{-x^2}x^{2n-1}\right]_{-\infty}^{\infty} + \frac{(2n-1)}{2}\int_{-\infty}^{\infty} dx e^{-x^2}x^{2n-2} \\
&= \frac{(2n-1)}{2}J_{n-1} \\
&= \frac{2n(2n-1)}{2^2 n}J_{n-1} \qquad n > 0 \qquad (3.8)
\end{aligned}$$

where we have used

$$\lim_{x\to\infty} x^n e^{-x^2} = \lim_{x\to\infty}\frac{x^n}{e^{x^2}} = \lim_{u\to\infty}\frac{u^{n/2}}{e^u} = \lim_{u\to\infty}\frac{u^{n/2}}{e^u} = \lim_{u\to\infty}\frac{\left(\frac{d}{du}\right)^m u^{n/2}}{e^u} = 0 \quad n > 0$$

where $m = n/2$ if $n$ is even and $n/2 + 1$ if $n$ is odd.

We calculate $J_0$ via the trick

$$\begin{aligned}
J_0^2 &= \int_{-\infty}^{\infty} dx e^{-x^2}\int_{-\infty}^{\infty} dy e^{-y^2} \\
&= \int_0^{2\pi} d\theta \int_0^{\infty} dr r e^{-r^2} \\
&= 2\pi\left[\frac{(-1)}{2}e^{-r^2}\right]_0^{\infty} \\
&= \pi.
\end{aligned}$$

Using $J_0 = \sqrt{\pi}$ with (3.8)

$$\begin{aligned}
J_n &= \frac{2n(2n-1)}{2^2 n}J_{n-1} \\
&= \frac{2n(2n-1)}{2^2 n}\frac{(2n-2)(2n-3)}{2^2(n-1)}J_{n-2} \\
&= \frac{2n(2n-1)}{2^2 n}\frac{(2n-2)(2n-3)}{2^2(n-1)}\cdots\frac{2\cdot 1}{2^2(2\cdot 1)}J_0 \\
&= \frac{(2n)!}{2^{2n}n!}\sqrt{\pi}. \qquad (3.9)
\end{aligned}$$

## 3.5 Method by Scaling trick

The integrals $I_n$ and $J_n$ can be found by a 'scaling' trick. Note

$$I(\alpha) = \int_0^\infty dx e^{-\alpha x} = \frac{1}{\alpha}\int_0^\infty dy e^{-y} = \frac{1}{\alpha}$$

where we have made the substitution $y = \alpha x$. And

$$J(\alpha) = \int_{-\infty}^\infty dx e^{-\alpha x^2} = \left[\frac{1}{\alpha}\right]^{\frac{1}{2}}\int_{-\infty}^\infty dy e^{-y^2} = \left[\frac{1}{\alpha}\right]^{\frac{1}{2}} J_0 = \left[\frac{\pi}{\alpha}\right]^{\frac{1}{2}}$$

where we have made the substitution $y = \sqrt{\alpha}x$. We can then easily find $I_n$ and $J_n$ by repeated differentiation with respect to $\alpha$ and then setting $\alpha = 1$, as such:

$$I_n = (-1)^n \left[\frac{d}{d\alpha}\right]^n I(\alpha)\Big|_{\alpha=1} \qquad J_n = (-1)^n \left[\frac{d}{d\alpha}\right]^n J(\alpha)\Big|_{\alpha=1}. \tag{3.10}$$

So that

$$I_n = (-1)^n \left[\frac{d}{d\alpha}\right]^n \frac{1}{\alpha}\bigg|_{\alpha=1} = \frac{n!}{\alpha^{n+1}}\bigg|_{\alpha=1} = n! \tag{3.11}$$

and

$$\begin{aligned}
J_n &= (-1)^n \left[\frac{d}{d\alpha}\right]^n \left[\frac{\pi}{\alpha}\right]^{\frac{1}{2}}\bigg|_{\alpha=1} \\
&= \frac{1}{2}\times\frac{3}{2}\times\cdots\times\frac{(2n-1)}{2}\,\frac{\sqrt{\pi}}{\alpha^{n+\frac{1}{2}}}\bigg|_{\alpha=1} \\
&= \frac{1\cdot 2\cdot 3\cdot 4\cdots(2n-1)\cdot 2n}{2^n(2\cdot 4\cdots 2n)}\sqrt{\pi} \\
&= \frac{(2n)!}{2^{2n}n!}\sqrt{\pi}. \qquad (3.12)
\end{aligned}$$

# Chapter 4

# Gram-Schmidt Orthogonalisation: Polynomial Bases

## 4.1 Introduction

Since at any particular stage of a Gram-Schmidt orthogonalisation we are dealing with a finite vector space, there are no problems generalising to function spaces.

We consider two examples in detail:

(i) Laguerre Polynomials, which sequentially orthogonalise the inner product:

$$(\psi_1, \psi_2) = \int_0^\infty dx e^{-x} \psi_1^*(x) \psi_2(x). \tag{4.1}$$

(ii) Hermite Polynomials, which sequentially orthogonalise the inner product:

$$(\psi_1, \psi_2) = \int_{-\infty}^\infty dx e^{-x^2} \psi_1^*(x) \psi_2(x). \tag{4.2}$$

We consider three 'techniques'

(a) Direct attack. ('Bull at a gate')

(b) Sneak attack.

(c) Foreknowledge.

We will be using Leibnitz's theorem, which we quote here

$$\left(\frac{d}{dx}\right)^n (uv) = \sum_{r=0}^{n} \frac{n!}{(n-r)!r!} \left(\frac{d}{dx}\right)^{n-r} (u) \left(\frac{d}{dx}\right)^{r} (v).$$

## 4.2 Direct Attack for Laguerre Polynomials

We orthogonalise $1, x, x^2, \ldots$ sequentially. We need

$$\int_0^\infty dx e^{-x} x^n = n!.$$

which we proved in the previous chapter.

Start with

$$P_0 = 1. \tag{4.3}$$

and write $P_1 = x - a_0$ (we are subtracting off an amount proportional to $P_0$) then

$$0 = (P_0, P_1) = \int_0^\infty dx e^{-x} P_0 P_1 = \int_0^\infty dx e^{-x}(x - a_0) = (1 - a_0)$$

implying $a_0 = 1$. So that

$$P_1 = x - 1. \tag{4.4}$$

Now we calculate $(P_1, P_1)$

$$(P_1, P_1) = \int_0^\infty dx e^{-x}(x-1)^2 = 2! - 2 + 1 = 1$$

We write $P_2 = x^2 - a_1(x-1) - a_0$ (we are subtracting off an amount proportional to $P_1$ and an amount proportional to $P_0$) then require

$$\begin{aligned} 0 = (P_0, P_2) &= \int_0^\infty dx e^{-x} P_0[x^2 - a_1 P_1 - a_0 P_0] \\ &= \int_0^\infty dx e^{-x} x^2 - a_0 = 2! - a_0 \end{aligned}$$

and

$$\begin{aligned} 0 = (P_1, P_2) &= \int_0^\infty dx e^{-x} P_1[x^2 - a_1 P_1 - a_0 P_0] \\ &= \int_0^\infty dx e^{-x}(x-1)x^2 - a_1 = 3! - 2! - a_1 = 4 - a_1. \end{aligned}$$

Giving $a_0 = 2$ and $a_1 = 4$. So that

$$P_2 = x^2 - 4x + 2. \tag{4.5}$$

.

Now we calculate $(P_2, P_2)$

$$\begin{aligned} (P_2, P_2) &= \int_0^\infty dx e^{-x}(x^2 - 4x + 2)(x^2 - 4P_1 + 2P_0) \\ &= \int_0^\infty dx e^{-x}(x^4 - 4x^3 + 2x^2) = 4! - 4 \cdot 3! + 2 \cdot 2 = 4 \end{aligned}$$

and so on...

## 4.3 Sneak Attack for Laguerre Polynomials

Consider

$$P_n(x) = e^x \left[\frac{d}{dx}\right]^n (e^{-x} x^n) \tag{4.6}$$

This useful choice of construction since by using integration by parts (we take $m \leq n$):

$$\begin{aligned} \int_0^\infty dx e^{-x} x^m P_n(x) &= \int_0^\infty dx x^m \left[\frac{d}{dx}\right]^n (e^{-x} x^n) \\ &= \left[x^m \left[\frac{d}{dx}\right]^{n-1} (e^{-x} x^n)\right]_0^\infty - \int_0^\infty dx \frac{d}{dx} x^m \left[\frac{d}{dx}\right]^{n-1} (e^{-x} x^n) \end{aligned} \tag{4.7}$$

We know from Leibnitz that the term $\left[\frac{d}{dx}\right]^{n-1}(e^{-x}x^n)$ is a sum of terms of the form $x^r e^{-x}$ for $r > 0$. These terms vanish when $x$ is put to zero, also from $\lim_{x\to\infty} x^r e^{-x} = 0$ they vanish for $x = \infty$, so the constant part vanishes in (4.7). After more integration by parts the constant part keeps zanishes for this same reason. After integrating by parts $n$ times (4.7) becomes

$$\begin{aligned}
\int_0^\infty dx e^{-x} x^m P_n(x) &= (-1)^n \int_0^\infty dx x^n e^{-x} \left[\frac{d}{dx}\right]^n x^m \\
&= \begin{cases} 0 & \text{for } m < n \\ (-1)^n (n!)^2 & \text{for } m = n \end{cases} \qquad (4.8)
\end{aligned}$$

This choice is orthogonal to all polynomials of degree less than $n$. With the use of Leibnitz's theorem, we easily see that $P_n(x)$ is a polynomial of degree $n$, and the coefficient of $x^n$ is just $(-1)^n$, so:

$$\begin{aligned}
\int_0^\infty dx e^{-x} P_n(x) P_m(x) &= \delta_{nm} \int_0^\infty dx e^{-x} P_n(x) P_n(x) \\
&= \delta_{nm} \int_0^\infty dx e^{-x} (-1)^n x^n P_n(x) \\
&= \delta_{nm} (n!)^2 \qquad (4.9)
\end{aligned}$$

where in the second line on the RHS we have used (4.8) for $m = n$, so that the normalised polynomials are just given by

$$\frac{1}{n!} e^x \left[\frac{d}{dx}\right]^n (e^{-x} x^n). \qquad (4.10)$$

Without the normalisation, these functions are know as the Laguerre Polynomials.

### 4.3.1 Explicit Formula for Laguerre Polynomials

It is easy to find an explicit form for general Laguerre polynomial using Leibnitz

$$\begin{aligned}
L_n(x) &= e^x \left[\frac{d}{dx}\right]^n (e^{-x} x^n) = e^x \sum_{k=0}^n \frac{n!}{k!(n-k)!} \left(\frac{d}{dx}\right)^k (x^n) \left(\frac{d}{dx}\right)^{n-k} e^{-x} \\
&= \sum_{k=0}^n (-1)^{n-k} \frac{n!}{k!(n-k)!} n \cdot (n-1) \cdot \ldots (n+1-k) x^{n-k} \\
&= \sum_{k=0}^n (-1)^{n-k} \frac{(n!)^2}{k![(n-k)!]^2} x^{n-k}. \qquad (4.11)
\end{aligned}$$

## 4.4 Foreknowledge for Laguerre Polynomials

$$\frac{e^{\frac{sx}{1-s}}}{1-s} = \sum_{n=0}^{\infty} \frac{s^n}{n!} P_n(x) \tag{4.12}$$

a generating function for Laguerre Polynomials. We come back to this in chapter 17.

## 4.5 Table of Laguerre Polynomials

We list the first few Laguerre polynomials, usually denoted $L_n(x)$:

$$\begin{aligned}
L_0(x) &= 1 \\
L_1(x) &= -x+1 \\
L_2(x) &= x^2-4x+2 \\
L_3(x) &= -x^3+9x^2-18x+6 \\
L_4(x) &= x^4-16x^3+72x^2-96x+24 \\
L_5(x) &= -x^5+25x^4-200x^3+600x^2-600x+120 \\
L_6(x) &= x^6-36x^5+450x^4-2400x^3+5400x^2-4320x+720.
\end{aligned} \tag{4.13}$$

if the reader wishes to verify them.

## 4.6 Direct Attack for Hermite Polynomials

We will need to know

$$\int_{-\infty}^{\infty} dx e^{-x^2} x^{2n} = \sqrt{\pi}\frac{(2n)!}{n!2^n}$$

which we proved in the previous chapter, and

$$\int_{-\infty}^{\infty} dx e^{-x^2} x^{2n+1} = 0$$

which follows from the integrand being an odd function, i.e. $e^{-x^2}(-x)^{2n+1} = -e^{-x^2}x^{2n+1}$.

Again we start with

$$P_0 = 1. \tag{4.14}$$

We calculate $(P_0, P_0)$,

$$(P_0, P_0) = \int_{-\infty}^{\infty} dx e^{-x^2} P_0^2 = \sqrt{\pi}.$$

We write $P_1 = x - a_0$ and require

$$0 = (P_0, P_1) = \int_{-\infty}^{\infty} dx e^{-x^2} P_0(x - a_0) = -a_0$$

implying $a_0 = 0$. so that

$$P_1 = x. \tag{4.15}$$

Now we calculate $(P_1, P_1)$,

$$(P_1, P_1) = \int_{-\infty}^{\infty} dx e^{-x^2} x^2 = \frac{\sqrt{\pi}}{2}$$

We write $P_2 = x^2 - a_1 x - a_0$ then require

$$\begin{aligned} 0 = (P_0, P_2) &= \int_{-\infty}^{\infty} dx e^{-x^2} P_0(x^2 - a_1 P_1 - a_0 P_0) \\ &= \frac{\sqrt{\pi}}{2} - a_0 \sqrt{\pi} \end{aligned}$$

and

$$\begin{aligned} 0 = (P_1, P_2) &= \int_{-\infty}^{\infty} dx e^{-x^2} P_1(x^2 - a_1 P_1 - a_0 P_0) \\ &= -a_1 \frac{\sqrt{\pi}}{2} \end{aligned}$$

Giving $a_0 = \frac{1}{2}$ and $a_1 = 0$. So that

$$P_2 = x^2 - \frac{1}{2}. \tag{4.16}$$

Now we calculate $(P_2, P_2)$

$$\begin{aligned}
(P_2, P_2) &= \int_{-\infty}^{\infty} dx e^{-x^2} (x^2 - \frac{1}{2})(x^2 - a_0 P_0) \\
&= \int_{-\infty}^{\infty} dx e^{-x^2} (x^4 - \frac{1}{2}x^2) \\
&= \frac{3\sqrt{\pi}}{4} - \frac{1}{2}\frac{\sqrt{\pi}}{2} \\
&= \frac{\sqrt{\pi}}{2}
\end{aligned}$$

and so on...

## 4.7 Sneak Attack for Hermite Polynomials

Consider

$$P_n(x) = e^{x^2} \left[\frac{d}{dx}\right]^n e^{-x^2} \tag{4.17}$$

The highest order term comes from the term that results from differentiates $e^{-x^2}$ the most times i.e. $(-1)^n (2x)^2$. Once again this is a clever choice, since:

Using integration by parts (we take $m \leq n$):

$$\begin{aligned}
\int_0^{\infty} dx e^{x^2} x^m P_n(x) &= \int_{-\infty}^{\infty} dx x^m \left[\frac{d}{dx}\right]^n e^{-x^2} \\
&= \left[ x^m \left[\frac{d}{dx}\right]^{n-1} (e^{-x^2}) \right]_{-\infty}^{\infty} - \int_0^{\infty} dx \frac{d}{dx} x^m \left[\frac{d}{dx}\right]^{n-1} (e^{-x^2})
\end{aligned} \tag{4.18}$$

We know that all the terms $\left[\frac{d}{dx}\right]^{n-1} e^{-x^2}$ is a sum of terms of the form $x^r e^{-x^2}$ for $r \geq 0$. These terms vanish when $x \to \pm\infty$ so part in big square brackets in (4.18) vanishes. After more integration by parts the square brackets keeps zanishes for this same reason. After integrating by parts $n$ times (4.18) becomes

$$\begin{aligned}
\int_{-\infty}^{\infty} dx e^{-x^2} x^m P_n(x) &= (-1)^n \int_0^{\infty} dx e^{-x^2} \left[\frac{d}{dx}\right]^n x^m \\
&= \left\{ \begin{array}{cl} 0 & \text{for} \quad m < n \\ (-1)^n n! \sqrt{\pi} & \text{for} \quad m = n \end{array} \right. \qquad (4.19)
\end{aligned}$$

This choice is orthogonal to all polynomials of degree less than $n$. So:

$$\begin{aligned}
\int_0^{\infty} dx e^{-x} P_n(x) P_m(x) &= \delta_{nm} \int_0^{\infty} dx e^{-x} P_n(x) P_n(x) \\
&= \delta_{nm} (-1)^n 2^n \int_0^{\infty} dx e^{-x} x^n P_n(x) \\
&= \delta_{nm} 2^n n! \sqrt{\pi} \qquad (4.20)
\end{aligned}$$

where in the second line on the RHS we have used (4.19) for $m = n$, so that the orthonormalised polynomials are just given by

$$\frac{(-1)^n}{\sqrt{2^n n! \sqrt{\pi}}} e^{x^2} \left[\frac{d}{dx}\right]^n e^{-x^2}. \qquad (4.21)$$

## 4.8 Foreknowledge for Hermite Polynomials

There is a generating function

$$e^{-t^2+2xt} = \sum_{n=0}^{\infty} \frac{t^n}{n!} P_n(x) \qquad (4.22)$$

for Hermite Polynomials. We come back to this in chapter 17.

## 4.9 Table of Hermite Polynomials

We list the first few Hermite polynomials, usually denoted $H_n(x)$,

$$
\begin{aligned}
H_0(x) &= 1 \\
H_1(x) &= 2x \\
H_2(x) &= 4x^2 - 2 \\
H_3(x) &= 8x^3 - 12x \\
H_4(x) &= 16x^4 - 48x^2 + 12 \\
H_5(x) &= 32x^5 - 160x^3 + 120x \\
H_6(x) &= 64x^6 - 480x^4 + 720x^2 - 120.
\end{aligned} \tag{4.23}
$$

if the reader wishes to verify them.

## 4.10 Note on Spanning the Vector Space

Note: We have now another demonstration that some function spaces - given polynomials of up to order $n$, there are always higer order polynomials as $x^{n+1}$ is linearly independent of lower order polynomials. We have an infinite number of orthogonal basis vectors. The current constructions provide a countable set (can be labelled by positive integers) of vectors, whether they span the space is a subtle issue! That is whether an arbitrary function in the space can be expanded in this basis is a subtle issue.

# Chapter 5

# Self-Adjoint Operators

## 5.1 Definition

The main thrust of the current analysis is to diagonalise operators in function spaces. The analogous results in finite-dimensional spaces corresponds to Hermitian operators, and so we need the function-space analogue to Hermitian: Self-adjoint.

A Hermitian operator on finite vector space is an operator such that $(\mathbf{x}, \hat{H}\mathbf{y}) = (\hat{H}\mathbf{x}, \mathbf{y})$ and so:

$$\int_a^b dx \psi_1^*(\hat{O}\psi_2)(x) = \int_a^b dx (\hat{O}\psi_1)^*(x)\psi_2(x) \tag{5.1}$$

is the analogue, known as self-adjoint. (NB: Note the weight function has been absorbed by the operator, $\hat{O}$)

## 5.2 Sturm-Liouville Theory

All the problems we will currently consider will be second order, so called Sturm-Liouville theory. We have a differential operator of the form:

$$\hat{O} = u_0(x)\frac{d^2}{dx^2} + u_1(x)\frac{d}{dx} + u_2(x). \tag{5.2}$$

Let us find out conditions for this operator to be self-adjoint. through integrating by parts we can move the operator over to $\psi_1^*$,

$$
\begin{aligned}
&\int_a^b dx\psi_1^*(x)(\hat{O}\psi_2)(x) = \int_a^b dx\psi_1^*(x)\left[u_2\psi_2 + u_1\frac{d\psi_2}{dx} + u_0\frac{d^2\psi_2}{dx^2}\right](x) \\
= &\left[u_1\psi_1^*\psi_2 + u_0\psi_1\frac{d\psi_2}{dx}\right]_a^b + \int_a^b dx\left[\psi_1^* u_2\psi_2 - \psi_2\frac{d}{dx}(u_1\psi_1^*) - \frac{d\psi_2}{dx}\frac{d}{dx}(u_0\psi_1^*)\right] \\
= &\left[u_1\psi_1^*\psi_2 + u_0\psi_1\frac{d\psi_2}{dx} - \psi_2\frac{d}{dx}(u_0\psi_1^*)\right]_a^b + \int_a^b dx\psi_2\left[u_2\psi_1^* - \frac{d}{dx}(u_1\psi_1^*) + \frac{d^2}{dx^2}(u_0\psi_1^*)\right] \\
= &\left[u_1\psi_1^*\psi_2 + u_0\psi_1\frac{d\psi_2}{dx} - \psi_2\frac{d}{dx}(u_0\psi_1^*)\right]_a^b + \int_a^b dx\psi_2(\hat{O}'\psi_1^*)(x) \qquad (5.3)
\end{aligned}
$$

where we have defined the operator $\hat{O}'$. For an operator to be self-adjoint we need a mixture of constraints on the functions $u_i(x)$ and boundary conditions.

Written out the operator $\hat{O}'$ is

$$
\hat{O}' = u_2 - \frac{du_1}{dx} + \frac{d^2u_0}{dx^2} + \left(2\frac{du_0}{dx} - u_1\right)\frac{d}{dx} + u_0\frac{d^2}{dx^2} \qquad (5.4)
$$

so for $\hat{O}' = \hat{O}$ we need

$$
u_2 - \frac{du_1}{dx} + \frac{d^2u_0}{dx^2} = u_2, \qquad 2\frac{du_0}{dx} - u_1 = u_1 \qquad (5.5)
$$

which are both simultaneously satisfied if:

$$
u_1(x) = \frac{du_0}{dx}(x). \qquad (5.6)
$$

We require the boundary conditions satify:

$$
\left[\left(u_1 - \frac{du_0}{dx}\right)\psi_1^*\psi_2 + u_0\left(\psi_1^*\frac{d\psi_2}{dx} - \psi_2\frac{d\psi_1^*}{dx}\right)\right]_a^b = 0
$$

and so we only need

$$
\left[u_0\left(\psi_1^*\frac{d\psi_2}{dx} - \psi_2\frac{d\psi_1^*}{dx}\right)\right]_a^b = 0 \qquad (5.7)
$$

if the previous condition (5.6) is satisfied.

Substituting (5.6) into (5.2) we find for $\hat{O}$ to be self-adjoint requires

$$\begin{aligned}\hat{O} &= u_0(x)\frac{d^2}{dx^2} + \frac{du_0}{dx}(x)\frac{d}{dx} + u_2(x) \\ &= \frac{d}{dx}\left[u_0(x)\frac{d}{dx}\right] + u_2(x).\end{aligned} \tag{5.8}$$

## 5.3 Construction of Self-Adjoint Operator

Given any $\hat{O}$ we can construct a self-adjoint operator (up to boundary conditions) by 'scaling'

Setting

$$\hat{O}' = v(x)\hat{O}$$

then $\hat{O}'$ is self-adjoint if:

$$\frac{d}{dx}(vu_0) = vu_1 = vu_0\frac{u_1}{u_0} \tag{5.9}$$

(in line with (5.6)) so

$$\frac{d}{dx}\ln(vu_0) = \frac{u_1}{u_0}$$

the solution of which is

$$vu_o = e^{\int^x dx' \frac{u_1}{u_0}(x')} \equiv A(x), \qquad \frac{dA}{dx}(x) = \frac{u_1}{u_0}A(x) = u_1 v \tag{5.10}$$

and in terms of

$$B(x) = u_2 v = \frac{u_2}{u_0}A(x) \tag{5.11}$$

we have

$$\begin{aligned}
\hat{O}' &= A(x)\frac{d^2}{dx^2} + \frac{dA}{dx}(x)\frac{d}{dx} + B(x) \\
&= \frac{d}{dx}\left[A(x)\frac{d}{dx}\right] + B(x)
\end{aligned} \tag{5.12}$$

(so of the form (5.8)) and

$$\begin{aligned}
\int_a^b dx\psi_1^*\left(\hat{O}'\psi_2\right) &= \int_a^b dxB(x)\psi_1^*\psi_2 + \int_a^b dx\psi_1^*\frac{d}{dx}\left(A(x)\frac{d\psi_2}{dx}\right) \\
&= \int_a^b dxB(x)\psi_1^*\psi_2 - \int_a^b dx\frac{d\psi_1^*}{dx}A(x)\frac{d\psi_2}{dx} + \left[A(x)\psi_1^*\frac{d\psi_2}{dx}\right]_a^b
\end{aligned} \tag{5.13}$$

and so $B(x)$ is a weight function and $A(x)$ is a sort of weight function for the derivatives. The boundary term usually vanishes.

### 5.3.1 Example 1: Rescale

We wish to rescale

$$\hat{O}(r) = -\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + 2r\frac{d}{dr} + 2 - \epsilon \tag{5.14}$$

into a self-adjoint form.

Now:

$$u_0(r) = (-1), \qquad u_1(r) = (-1)\frac{1}{r} + 2r, \qquad u_2(r) = 2 - \epsilon$$

so:

$$\begin{aligned}
A(r) &= \exp\left[\int^r dr'\left[\frac{1}{r'} + 2r'\right]\right] \\
&= \exp\left(\ln r - r^2\right) \\
&= re^{-r^2}
\end{aligned} \tag{5.15}$$

and

$$B(r) = \frac{u_2}{u_0} A(r) = (\epsilon - 2) r e^{-r^2} \tag{5.16}$$

and then, including a minus sign:

$$\hat{O}(r) \mapsto -\frac{d}{dr}\left[ r e^{-r^2} \frac{d}{dr} \right] + (2 - \epsilon) r e^{-r^2}. \tag{5.17}$$

### 5.3.2 Example 2: Rescale

We wish to rescale

$$\hat{T}(x) = (1 - x^2)\frac{d^2}{dx^2} - x\frac{d}{dx} + n^2 \tag{5.18}$$

into a self-adjoint form.

Now:

$$u_0(x) = 1 - x^2, \qquad u_1(x) = -x, \qquad u_2(x) = n^2$$

so:

$$\begin{aligned} A(x) &= \exp\left[ \int^x dx' \frac{-x'}{1 - x'^2} \right] \\ &= \exp\left[ \frac{1}{2} \ln(1 - x^2) \right] \\ &= (1 - x^2)^{\frac{1}{2}} \end{aligned} \tag{5.19}$$

and

$$B(x) = \frac{u_2(x)}{u_0(x)} A(x) = \frac{n^2}{(1 - x^2)^{\frac{1}{2}}} \tag{5.20}$$

and then:

$$T(x) \mapsto \frac{d}{dx}\left[(1-x^2)^{\frac{1}{2}}\frac{d}{dx}\right] + \frac{n^2}{(1-x^2)^{\frac{1}{2}}}. \tag{5.21}$$

Let us look at our previous work in this context.

# Chapter 6

# Laguerre Polynomials

Recall we can obtain Laguerre Polynomials via

$$L_n(x) = e^x \left[\frac{d}{dx}\right]^n (e^{-x}x^n). \tag{6.1}$$

In Eigenphysics I, section 15.2 we proved from this that $L_n(x)$ satisfies the differential equation

$$x\frac{d^2 L_n}{dx^2} + (1-x)\frac{dL_n}{dx} + nL_n = 0 \tag{6.2}$$

Let us make this operator self-adjoint. Now:

$$u_0(x) = x, \qquad u_1(x) = (1-x), \qquad u_2(x) = n$$

so:

$$\begin{aligned} A(x) &= \exp\left[\int^x dx' \frac{(1-x')}{x'}\right] \\ &= \exp[\ln x - x] \\ &= xe^{-x} \end{aligned} \tag{6.3}$$

and

$$B(x) = \frac{u_2}{u_0} A(x) = ne^{-x} \tag{6.4}$$

and then

$$\hat{O} = \frac{d}{dx}\left[xe^{-x}\frac{d}{dx}\right] + ne^{-x}. \tag{6.5}$$

is a self-adjoint operator. The weight function $e^{-x}$ was previously used to orthonormalise polynomials when constructing these objects.

Note the equation:

$$\hat{O}L_n(x) = 0 \tag{6.6}$$

reduces to (6.2).

# Chapter 7

# Hermite Polynomials

Recall we can obtain Hermite Polynomials via

$$H_n(x) = e^{x^2} \left[\frac{d}{dx}\right]^n e^{-x^2}. \tag{7.1}$$

We first write

$$\frac{d}{dx} e^{-x^2} + 2x e^{-x^2} = 0 \tag{7.2}$$

and set

$$H_n' = e^{-x^2} H_n = \left[\frac{d}{dx}\right]^n e^{-x^2}$$

In (7.2) we have a factor proportional to $x$, in this case (i.e. $xf(x)$) Leibnitz reduces to

$$\left(\frac{d}{dx}\right)^n (f(x)x) = x \left(\frac{d}{dx}\right)^n f(x) + n \left(\frac{d}{dx}\right)^{n-1} f(x).$$

Applying $\left(\frac{d}{dx}\right)^{n+1}$ to (7.2) we obtain from Leibnitz

$$\begin{aligned}
& \left(\frac{d}{dx}\right)^{n+1} \left[\frac{d}{dx} e^{-x^2} + 2x e^{-x^2}\right] \\
= \; & \frac{d^2}{dx^2} \left(\frac{d}{dx}\right)^n e^{-x^2} + 2x \frac{d}{dx} \left(\frac{d}{dx}\right)^n e^{-x^2} + 2(n+1) \left(\frac{d}{dx}\right)^n e^{-x^2} \\
= \; & \frac{d^2 H_n'}{dx^2} + 2x \frac{dH_n'}{dx} + 2(n+1) H_n' = 0
\end{aligned} \tag{7.3}$$

Using Leibnitz we have

$$\frac{d^2}{dx^2}[e^{-x^2}H_n] = e^{-x^2}\frac{d^2H_n}{dx^2} - 4xe^{-x^2}\frac{dH_n}{dx} + (4x^2-2)e^{-x^2}H_n$$

and

$$\frac{d}{dx}[e^{-x^2}H_n] = e^{-x^2}\frac{dH_n}{dx} - 2xe^{-x^2}H_n.$$

Substituting these into the last line of (7.3) and multiplying by $e^{x^2}$ we obtain

$$\left(\frac{d^2H_n}{dx^2} - 4x\frac{dH_n}{dx} + (4x^2-2)H_n\right) + 2x\left(\frac{dH_n}{dx} - 2xH_n\right) + 2(n+1)H_n = 0 \tag{7.4}$$

This simplifies to

$$\frac{d^2H_n}{dx^2} - 2x\frac{dH_n}{dx} + 2nH_n = 0. \tag{7.5}$$

Once again we make this operator self-adjoint. Now:

$$u_0(x) = 1, \qquad u_1(x) = -2x, \qquad u_2(x) = 2n$$

so:

$$\begin{aligned} A(x) &= \exp\left[\int^x dx'(-2)x'\right] \\ &= e^{-x^2} \end{aligned} \tag{7.6}$$

and

$$B(x) = \frac{u_2}{u_0}A(x) = 2ne^{-x^2} \tag{7.7}$$

and the self-adjoint operator is

$$\hat{O} = \frac{d}{dx}\left[e^{-x^2}\frac{d}{dx}\right] + 2ne^{-x^2}. \tag{7.8}$$

The weight function $e^{-x^2}$ was previously used to orthonormalise polynomials when constructing these objects.

Note the equation:

$$\hat{O}H_n(x) = 0 \tag{7.9}$$

reduces to (7.5).

# Chapter 8

# Sturm-Liouville Theory

Self-adjoint operators are analogous to Hermitian operators, and the analogous problem to diagalisation is to solve the Sturm-Liouville problem:

$$\hat{L}\phi(x) = \epsilon w(x)\phi(x) \tag{8.1}$$

for eigenvalues, $\epsilon$, and eigenfunctions $\phi(x)$, where $\hat{L}$ has the form

$$\hat{L} = \frac{d}{dx}\left[p(x)\frac{d}{dx}\right] + q(x). \tag{8.2}$$

The $w(x)$ is the weight function, the corresponding inner product is:

$$(\psi_1, \psi_2) = \int_a^b dx w(x)\psi_1^*(x)\psi_2(x) \tag{8.3}$$

and $\hat{L}$ is a self-adjoint operator.

## 8.1 Examples

We already have two such problems solved:

(i) $w(x) = e^{-x}$,

$$\hat{L} = -\frac{d}{dx}\left[e^{-x}x\frac{d}{dx}\right] \tag{8.4}$$

and then

$$\hat{L}L_n(x) = ne^{-x}L_n(x) \tag{8.5}$$

is satisfied by the Laguerre polynomials

$$L_n(x) = e^x \left[\frac{d}{dx}\right]^n (e^{-x}x^n)$$

as (8.4) and (8.5) combine to give

$$-\frac{d}{dx}\left[e^{-x^2}x\frac{d}{dx}\right]L_n(x) = ne^{-x}L_n(x)$$

which is equivalent to (6.6) that reduces to the differential equaiotn for Laguerre polynomials. So $L_n(x)$ is an eigenfunction with eigenvalue, $\epsilon_n = n$, with integral $n$.

(ii) $w(x) = e^{-x^2}$,

$$\hat{L} = -\frac{d}{dx}\left[e^{-x^2}\frac{d}{dx}\right] \tag{8.6}$$

and then

$$\hat{L}H_n(x) = 2ne^{-x^2}H_n(x) \tag{8.7}$$

is satisfied by the Hermite polynomials

$$H_n(x) = (-1)^n e^{x^2}\left[\frac{d}{dx}\right]^n (e^{-x^2})$$

as (8.6) and (8.7) combine to give

$$-\frac{d}{dx}\left[e^{-x^2}\frac{d}{dx}\right]H_n(x) = 2ne^{-x^2}H_n(x)$$

which is equivalent to (7.9) that reduces to the differential equaiotn for Hermite polynomials. So $H_n(x)$ is an eigenfunction with eigenvalue, $\epsilon_n = 2n$, with integral $n$.

## 8.2 Equivalent Optimising Problem

Define $\hat{L}' = \frac{1}{w(x)}\hat{L}$. Consider

$$
\begin{aligned}
F[\psi^*, \psi(x)] &= \frac{(\psi, \hat{L}'\psi)}{(\psi, \psi)} \\
&= \frac{\int_a^b dx\psi^*(x)\left(\frac{d}{dx}\left[p(x)\frac{d\psi(x)}{dx}\right] + q(x)\psi(x)\right)}{\int_a^b dx w(x)\psi^*(x)\psi(x)}
\end{aligned}
\tag{8.8}
$$

Which is the same as minimising

$$
\int_a^b dx\psi^*(x)\left(\frac{d}{dx}\left[p(x)\frac{d\psi(x)}{dx}\right] + q(x)\psi(x)\right) \equiv \int_a^b dx\mathcal{L}(x)
$$

subject to the constraint

$$
\int_a^b dx w(x)\psi^*(x)\psi(x) = 1.
$$

We do this by substituting $\mathcal{L}$ into

$$
\frac{\partial \mathcal{L}}{\partial \psi^*} - \epsilon \frac{\partial}{\partial \psi^*}[w\psi^*\psi] = 0
$$

where $\epsilon$ is a Lagrangian multiplier. Which gives

$$
\frac{d}{dx}\left[p(x)\frac{d\psi(x)}{dx}\right] + q(x)\psi(x) = \epsilon w\psi. \tag{8.9}
$$

## 8.3 Theorems

(i) Eigenvalues are real.

(ii) Non-degenerate eigenfunctions are orthogonal.

If $\hat{L}\psi_n = \epsilon_n w\psi_n$, i.e. $\hat{L}'\psi_n = \epsilon_n\psi_n$, then

$$\epsilon_n(\psi_m, \psi_n) = (\psi_m, \hat{L}'\psi_n) = (\hat{L}'\psi_m, \psi_n) = \epsilon_m^*(\psi_m, \psi_n) \tag{8.10}$$

and so

$$(\epsilon_n - \epsilon_m^*)(\psi_m, \psi_n) = 0. \tag{8.11}$$

(a) If $n = m$ then $(\psi_n, \psi_n) > 0$ implies to $\epsilon_n = \epsilon_n^*$ and the eigenvalues are real.

(b) If $n \neq m$ and $\epsilon_n \neq \epsilon_m$ then $(\psi_m, \psi_n) = 0$ and the eigenfunctions are necessarily orthogonal.

Note: We used the orthogonalisation idea to construct our current polynomials.

# Chapter 9

# Fourier Series

## 9.1 First Boundary Conditions

A very simple example of a Sturn-Lioville problem is:

$$\hat{L} = -\frac{d^2}{dx^2} \tag{9.1}$$

for $x \in (0, 1)$, combined with the boundary condition that $\psi(0) = 0 = \psi(1)$, and uniform weight $w = 1$. This is self-adjoint as it is of the form (5.8) and the boundary condition (5.7)

$$\left[(-1)\left(\psi_1^* \frac{d\psi_2}{dx} - \psi_2 \frac{d\psi_1^*}{dx}\right)\right]_0^1 = 0$$

is obviously satisfied.

The diagonalisation of this operator is equivalent to finding a fourier series. Diagonalisation corresponds to solving the Sturm-Liouville problem, namely (8.1):

$$-\frac{d^2\psi}{dx^2} = \epsilon\psi \tag{9.2}$$

which solves to give

$$\psi(x) = A\sin(\sqrt{\epsilon}x + a) \qquad \epsilon > 0. \tag{9.3}$$

Imposing $\psi(0) = 0 = \psi(1)$ implies $A \sin a = 0$ and $A\sin(\sqrt{\epsilon} + a)$, and so $a = 0$ and $\sqrt{\epsilon} = n\pi$ for $n = 1, 2, \dots$ . The constant $A$ is determined by normalisation:

$$
\begin{aligned}
1 &= A^2 \int_0^1 dx \sin^2(n\pi x) \\
&= A^2 \left[ \frac{\cos(n\pi x)}{n\pi} \sin(n\pi x) \right]_0^1 + A^2 \int_0^1 dx \cos^2(n\pi x) \\
&= A^2 \frac{1}{2} \int_0^1 dx \left( \sin^2(n\pi x) + \cos^2(n\pi x) \right) = A^2 \frac{1}{2}.
\end{aligned}
$$

The eigenfunctions are then:

$$\psi(x) = \sqrt{2} \sin(n\pi x) \tag{9.4}$$

with eigenvalues,

$$\epsilon = n^2 \pi^2. \tag{9.5}$$

Expanding any function which vanishes at $x = 0$ and 1 in a fourier series is equivalent to diagonalising $-\frac{d^2}{dx^2}$.

## 9.2 Second Boundary Conditions

A second very natural boundary condition is that of periodic boundary conditions:

$$\psi(x + 2\pi) = \psi(x), \tag{9.6}$$

and then we are dealing with a true angle $x \mapsto \phi$.

# Chapter 10

# Discontinuities

For this section you will need to remember the definition of $\delta-$functions and step functions $\Theta$:

$$\int^{x} dy \delta(y) = \Theta(x)$$

$\delta(x)$ has unit area but all 'infinitesimally' close to $x = 0$ and $\Theta(x)$ vanishes when $x < 0$ and takes the valueunity when $x > 0$.

Sometimes we want to think about functions with 'discontinuities'. For a Sturm-Lioville problem we can consider functions with discontinuous slope or smoother, but nothing worse.

If

$$\hat{L} = -\frac{d}{dx}\left[a(x)\frac{d}{dx}\right] \tag{10.1}$$

then

$$\begin{aligned} \int_a^b dx \psi_1^* \hat{L} \psi_2 &= -\int_a^b dx \psi_1^* \frac{d}{dx}\left[a(x)\frac{d}{dx}\right] \\ &= \left[-\psi_1^* a \frac{d\psi_2}{dx}\right]_a^b + \int_a^b dx a(x) \frac{d\psi_1^*}{dx}\frac{d\psi_2}{dx}. \end{aligned} \tag{10.2}$$

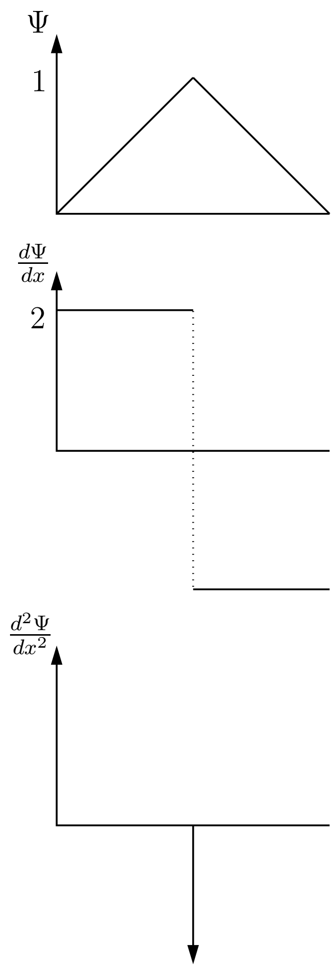
Providing that the boundary-term vanishes, we can represent $\hat{L}$ in terms of first derivatives of $\psi$. We can handle discontinuities in $\frac{d\psi}{dx}$, even though $\frac{d^2\psi}{dx^2}$ is divergent.

Example:

$$\psi(x) = 2x\Theta(\frac{1}{2} - x) + (2 - 2x)\Theta(x - \frac{1}{2}) \tag{10.3}$$

$$\frac{d\psi}{dx}(x) = 2\Theta(\frac{1}{2} - x) - 2\Theta(x - \frac{1}{2}) \tag{10.4}$$

$$\frac{d^2\psi}{dx^2} = -4\delta(x - \frac{1}{2}) \tag{10.5}$$




The moral to this story is always use the single-derivative form of the operator. Any calculation will be simplified!

# Chapter 11

# Variational Calculations

If we desire the lowest energy eigenvalue, then we can obtain upper bounds forit by using 'trial wavefunctions'. The idea is that

$$\epsilon_0 \leq \frac{(\psi, \hat{L}'\psi)}{(\psi, \psi)} \tag{11.1}$$

where $\epsilon_0$ is the ground state energy and $\psi$ is an arbitrary wavefunction. Clever choices of $\psi$ can give very good estimates.

'**Proof**': If the eigenfunctions $\psi_n$ form a basis for our vector space, then any $\psi$ can be expanded as

$$\psi = \sum_{n=0}^{\infty} a_n \psi_n \tag{11.2}$$

and so

$$\hat{L}'\psi = \sum_{n=0}^{\infty} a_n \hat{L}'\psi_n = \sum_{n=0}^{\infty} a_n \epsilon_n \psi_n.$$

Substituiting this into $(\psi, \hat{L}'\psi)$ we obtain

$$
\begin{aligned}
(\psi, \hat{L}'\psi) &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}(a_m\psi_m, a_n\epsilon_n\psi_n) \\
&= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} a_m^* a_n \epsilon_n(\psi_m, \psi_n) \\
&= \sum_{m=0}^{\infty} a_n^* a_n \epsilon_n \qquad (11.3)
\end{aligned}
$$

where we have used $(\psi_m, \psi_n) = \delta_{mn}$, and then substituiting it into $(\psi, \psi)$ we find

$$
\begin{aligned}
(\psi, \psi) &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty}(a_m\psi_m, a_n\psi_n) \\
&= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} a_m^* a_n(\psi_m, \psi_n) \\
&= \sum_{m=0}^{\infty} a_n^* a_n \qquad (11.4)
\end{aligned}
$$

Now by definition of $\epsilon_0$, $\epsilon_n \geq \epsilon_0$ so

$$a_n^* a_n \epsilon_n \geq \epsilon_0 a_n^* a_n, \qquad (11.5)$$

summing over $n$ gives

$$\sum_{n=0}^{\infty} a_n^* a_n \epsilon_n \geq \epsilon_0 \sum_{n=0}^{\infty} a_n^* a_n$$

which gives the desired result

$$\epsilon_0 \leq \frac{\sum_{n=0}^{\infty} a_n^* a_n \epsilon_n}{\sum_{n=0}^{\infty} a_n^* a_n} = \frac{(\psi, \hat{L}'\psi)}{(\psi, \psi)}. \qquad (11.6)$$

we find strict equality if (11.5) holds for all $n$, that is if $a_n^* a_n(\epsilon_n - \epsilon_0) = 0$ for all $n$, i.e. if we are in the ground-state subspace.

## 11.1 Example:

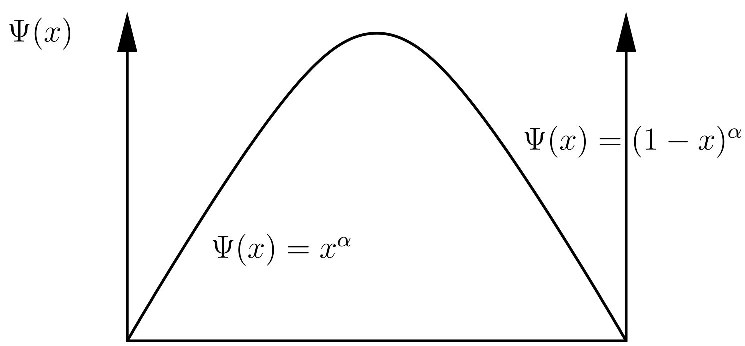
We will look at various trial wavefunctions for $\hat{L} = -\frac{d^2}{dx^2}$ on the interval $x \in (0, 1)$ with uniform weight function and $\psi(0) = 0 = \psi(1)$. We already know that the ground state is:

$$\psi_0 = \sqrt{2} \sin \pi x$$

with eigenvalue $\epsilon_0 = \pi^2$.

### 11.1.1 First Trial Function

Try




Note the discontinuity in slope at $x = \frac{1}{2}$. Use

$$\epsilon_0 \leq \frac{(\psi, \hat{L}\psi)}{(\psi, \psi)} = \frac{\int_0^1 dx \left[\frac{d\psi}{dx}\right]^2}{\int_0^1 dx[\psi]^2}.$$

By symmetry, we can consider only the first half. $\psi = x^\alpha$ and $\frac{d\psi}{dx} = \alpha x^{\alpha-1}$, so

$$\int_0^{1/2} dx \psi^2 = \int_0^{1/2} dx x^{2\alpha} = \frac{1}{2\alpha+1}\left(\frac{1}{2}\right)^{2\alpha+1}$$

$$\int_0^{1/2} dx \left[\frac{d\psi}{dx}\right]^2 = \alpha^2 \int_0^{1/2} dx x^{2\alpha-2} = \frac{\alpha^2}{2\alpha-1}\left(\frac{1}{2}\right)^{2\alpha-1}$$

so

$$\epsilon_0 \leq \frac{4\alpha^2(2\alpha+1)}{(2\alpha-1)} = \frac{1}{\beta}(\beta+2)(\beta+1)^2$$

in terms of $\beta = 2\alpha - 1$. To find the best bound, we can minimise over $\beta$.

$$\frac{\partial}{\partial\beta}\left[\beta^2 + 4\beta + 5 + \frac{2}{\beta}\right] = 2\beta + 4 - \frac{2}{\beta^2} = 0$$

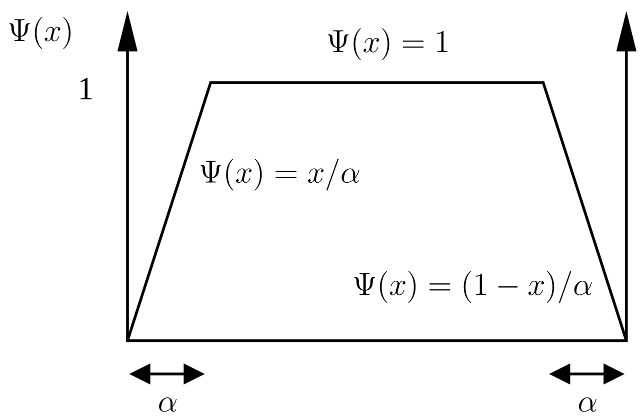
so $\beta^3 + 2\beta^2 - 1 = (\beta+1)(\beta^2+\beta-1) = 0$ and the relevant root is $\beta = \frac{\sqrt{5}-1}{2}$ and $\alpha = \frac{\sqrt{5}-+1}{2}$, and substituting in yields $\beta = 0.618034$, $\alpha = 0.809017$ and

$$\epsilon_0 \leq \epsilon = \frac{11 + 5\sqrt{5}}{2} = 11.090170.$$

All that work and not very close to the exact solution of $\epsilon_0 = \pi^2 = 9.8696044$.

### 11.1.2 Second Trial Function

Try




Once again, discontinuties and symmetry about $x = \frac{1}{2}$.

$$\int_0^{1/2} dx\psi^2 = \int_0^{\alpha} dx\frac{x^2}{\alpha^2} + \int_{\alpha}^{1/2} dx = \frac{\alpha}{3} + \frac{1}{2} - \alpha = \frac{1}{2} - \frac{2\alpha}{3}$$

$$\int_0^{1/2} dx\left[\frac{d\psi}{dx}\right]^2 = \int_0^{\alpha} dx\frac{1}{\alpha^2} = \frac{1}{\alpha}$$

so

$$\epsilon_0 \leq \frac{1}{\alpha\left[\frac{1}{2} - \frac{2\alpha}{3}\right]} = \frac{6}{\alpha(3 - 4\alpha)}$$

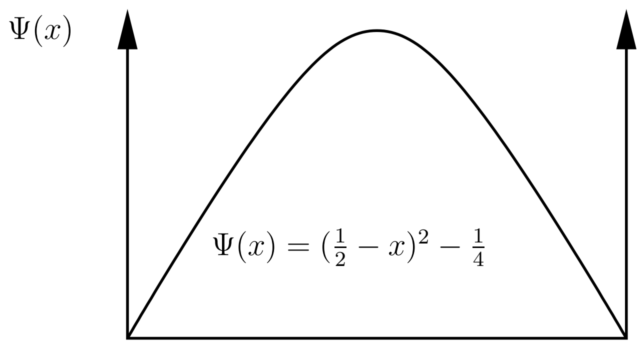
the final minimisation over $\alpha$ leads to

$$\frac{\partial}{\partial\alpha}[\alpha(3-4\alpha)] = 3 - 8\alpha = 0$$

so $\alpha = \frac{3}{8} = 0.375$ and $\epsilon_0 \leq \epsilon = \frac{32}{3} = 10.66...$ Better than before, but that before, but still not good.

### 11.1.3 Third Trial Function

Try




A quadratic equation $\left(\frac{1}{2} - x\right)^2 - \frac{1}{4} = x^2 - x$, and $\frac{d\psi}{dx} = 2x - 1$. This function has no free parameters, so at first sight it might appear a poor choice.

$$\int_0^1 dx\psi^2 = \int_0^1 dx(x-1)^2x^2 = \int_0^1 dx(x^2 - 2x^3 + x^4) = \frac{1}{3} - \frac{2}{4} + \frac{1}{5} = \frac{10-15+6}{30} = \frac{1}{30}$$

$$\int_0^{1/2} dx\left[\frac{d\psi}{dx}\right]^2 = \int_0^1 dx(2x-1)^2 = \int_0^1 dx(1 - 4x + 4x^2) = 1 - \frac{4}{2} + \frac{4}{3} = \frac{1}{3}$$

so $\epsilon_0 \leq \frac{1/3}{1/30} = 10$. Really quite good, and no variational parameter.

### 11.1.4 Fourth Trial Function

Try

$$\psi(x) = (2x-1)^4 + \alpha(2x-1)^2 - 1 - \alpha$$

$$\frac{d\psi}{dx} = 8(2x-1)^3 + 4\alpha(2x-1)$$

a generalisation of the previous try. Reparametrise $z = 2x - 1$ to provide:

$$\begin{aligned}
&\int_{1/2}^{1} dx\psi^2 = \int_0^1 \frac{dz}{2}[z^4 + \alpha z^2 - 1 - \alpha]^2 \\
&= \int_0^1 \frac{dz}{2}[(1+\alpha)^2 - 2\alpha(1+\alpha)z^2 + (\alpha^2 - 2\alpha - 2)z^4 + 2\alpha z^6 + z^8] \\
&= \frac{1}{2}\left[(1+\alpha)^2 - 2\alpha(1+\alpha)\frac{1}{3} + (\alpha^2 - 2\alpha - 2)\frac{1}{5} + 2\alpha\frac{1}{7} + \frac{1}{9}\right] \\
&= \frac{1}{2}\left[\alpha^2(1 - \frac{2}{3} + \frac{1}{5}) + \alpha(2 - \frac{2}{3} - \frac{2}{5} + \frac{2}{7}) + (1 - \frac{2}{5} + \frac{1}{9})\right] \\
&= \frac{1}{2}\left[\frac{8\alpha^2}{15} + \frac{128\alpha}{105} + \frac{32}{45}\right]
\end{aligned}$$

$$\int_0^{1/2} dx \left[\frac{d\psi}{dx}\right]^2 = \int_0^1 \frac{dz}{2} 16z^2(\alpha + 2z^2)^2 = \frac{16}{2}\left[\alpha^2\frac{1}{3} + 4\alpha\frac{1}{5} + 4\frac{1}{7}\right]$$

so

$$\begin{aligned}
\epsilon_0 \le \epsilon &= \frac{16\left[\frac{\alpha^2}{3} + \frac{4\alpha}{5} + \frac{4}{7}\right]}{\left[\frac{8\alpha^2}{15} + \frac{128\alpha}{105} + \frac{32}{45}\right]} = \frac{(3 \times 105/8) \times 16[\frac{\alpha^2}{3} + \frac{4\alpha}{5} + \frac{4}{7}]}{3 \times 105/8[\frac{8\alpha^2}{15} + \frac{128\alpha}{105} + \frac{32}{45}]} \\
&= \frac{2[105\alpha^2 + 252\alpha + 180]}{[21\alpha^2 + 48\alpha + 28]} \\
&= 10 + \frac{2[(252 - 240)\alpha + (180 - 140)]}{[21\alpha^2 + 48\alpha + 28]} \\
&= 10 + \frac{3\alpha + 10}{[21\alpha^2 + 48\alpha + 28]}
\end{aligned} \tag{11.7}$$

minimising

$$\frac{\partial}{\partial\alpha}\frac{3\alpha + 10}{[21\alpha^2 + 48\alpha + 28]} = 0$$

yields

$$3[21\alpha^2 + 48\alpha + 28] - (3\alpha + 10)[42\alpha + 48] = -3[21\alpha^2 + 140\alpha + 132] = 0$$

and

$$\left(\alpha+\frac{10}{3}\right)^2-\frac{100}{9}+\frac{132}{21}=\left(\alpha+\frac{10}{3}\right)^2-\frac{304}{63}=0$$

so

$$\alpha=-\frac{10}{3}-\left[\frac{304}{63}\right]^{1/2}=-5.530012$$

and $\epsilon_0 \leq \epsilon = 9.869750$ good to several decimal places.

# Chapter 12

# Exercise: Chebychev's Polynomials

## 12.1 Exercise

Test your understanding on the following example, show that:

(i) the functions defined by

$$T_n(x) = [1 - x^2]^{\frac{1}{2}} \left[\frac{d}{dx}\right]^n [1 - x^2]^{n-\frac{1}{2}} \tag{12.1}$$

provide an orthonormal basis for inner product:

$$\int_{-1}^{1} \frac{dx}{[1 - x^2]^{\frac{1}{2}}} T_1^*(x) T_2(x). \tag{12.2}$$

(ii) Show that the $T_n(x)$ satisfy:

$$(1 - x^2)\frac{d^2T_n}{dx^2} - x\frac{dT_n}{dx} + n^2 T_n = 0. \tag{12.3}$$

(iii) Find the self-adjoint representation for the Sturm-Liouville operator and verify that:

$$\hat{T}(x) T_n(x) = \frac{n^2}{[1 - x^2]^{\frac{1}{2}}} T_n(x) \tag{12.4}$$

for a particular choice.

(iv) Show that this problem is related to a Fourier series problem.

**Solution**.

(i) We use (12.1) to abtain the firsy few polynomials:

$$T_0(x) = 1$$

$$\begin{aligned} T_1(x) &= [1-x^2]^{\frac{1}{2}} \left[\frac{d}{dx}\right] [1-x^2]^{\frac{1}{2}} \\ &= -[1-x^2]^{\frac{1}{2}}(x[1-x^2]^{-\frac{1}{2}}) \\ &= (-1)x. \end{aligned} \tag{12.5}$$

$$\begin{aligned} T_2(x) &= [1-x^2]^{\frac{1}{2}} \left[\frac{d}{dx}\right]^2 [1-x^2]^{\frac{3}{2}} \\ &= -3[1-x^2]^{\frac{1}{2}} \left[\frac{d}{dx}\right] (x[1-x^2]^{\frac{1}{2}}) \\ &= -3[1-x^2]^{\frac{1}{2}}([1-x^2]^{\frac{1}{2}} - x^2[1-x^2]^{-\frac{1}{2}}) \\ &= -3([1-x^2] - x^2) \end{aligned} \tag{12.6}$$

$$\begin{aligned} T_3(x) &= [1-x^2]^{\frac{1}{2}} \left[\frac{d}{dx}\right]^3 [1-x^2]^{\frac{5}{2}} \\ &= -5[1-x^2]^{\frac{1}{2}} \left[\frac{d}{dx}\right]^2 (x[1-x^2]^{\frac{3}{2}}) \\ &= -5[1-x^2]^{\frac{1}{2}} \left[\frac{d}{dx}\right] \left([1-x^2]^{\frac{3}{2}} - 3x^2[1-x^2]^{\frac{1}{2}}\right) \\ &= (-5)\left((-3)x[1-x^2] - 6x[1-x^2] + 3x^3\right) \end{aligned} \tag{12.7}$$

and so on. We wish to find the general expression for the coefficient of the $x^n$ term of $T_n(x)$. For $n$ even:

$$
\begin{aligned}
T_n(x) &= [1-x^2]^{\frac{1}{2}} \left[\frac{d}{dx}\right]^n [1-x^2]^{n-\frac{1}{2}} \\
&= -(2n-1)[1-x^2]^{\frac{1}{2}} \left[\frac{d}{dx}\right]^{n-1} (x[1-x^2]^{n-1-\frac{1}{2}}) \\
&= -(2n-1)[1-x^2]^{\frac{1}{2}} \left[\frac{d}{dx}\right]^{n-1} ([1-x^2]^{n-1-\frac{1}{2}}) + \dots \\
&= (-1)^{\frac{n}{2}}(2n-1)(2n-3)\dots(2n-[n-1])([1-x^2]^{\frac{n}{2}}) + \dots \\
&= (-1)^n(2n-1)(2n-3)\dots(n+1)\frac{n}{2}x^n + \dots \qquad (12.8)
\end{aligned}
$$

For $n$ odd:

$$
\begin{aligned}
T_n(x) &= [1-x^2]^{\frac{1}{2}} \left[\frac{d}{dx}\right]^n [1-x^2]^{n-\frac{1}{2}} \\
&= -(2n-1)[1-x^2]^{\frac{1}{2}} \left[\frac{d}{dx}\right]^{n-1} (x[1-x^2]^{n-1-\frac{1}{2}}) \\
&= -(2n-1)[1-x^2]^{\frac{1}{2}} \left[\frac{d}{dx}\right]^{n-1} ([1-x^2]^{n-1-\frac{1}{2}}) + \dots \\
&= (-1)^{\frac{n-1}{2}}(2n-1)(2n-3)\dots(2n-n)(x[1-x^2]^{\frac{n-1}{2}}) + \dots \\
&= (-1)^n(2n-1)(2n-3)\dots n\frac{n-1}{2}x^n + \dots \qquad (12.9)
\end{aligned}
$$

$$
c_n = (-1)^n 2^{n-1} \qquad (12.10)
$$

We now prove that the Chebyshev polynomials are orthogonal. Assume that $m \leq n$ and consider

$$
\begin{aligned}
\int_{-1}^{1} \frac{dx}{[1-x^2]^{\frac{1}{2}}} x^m T_n(x) &= \int_{-1}^{1} dx x^m \left[\frac{d}{dx}\right]^n [1-x^2]^{n-\frac{1}{2}} \\
&= \left[x^m \left[\frac{d}{dx}\right]^{n-1} [1-x^2]^{n-\frac{1}{2}}\right]_{-1}^{1} - \int_{-1}^{1} dx \frac{d}{dx} x^m \left[\frac{d}{dx}\right]^{n-1} [1-x^2]^{n-\frac{1}{2}}
\end{aligned} \qquad (12.11)
$$

After integrating by parts another $n-1$ times (12.11) becomes

$$\int_{-1}^{1} \frac{dx}{[1-x^2]^{\frac{1}{2}}} x^m T_n(x) = (-1)^n \int_{-1}^{1} dx[1-x^2]^{n-\frac{1}{2}} \left[\frac{d}{dx}\right]^n x^m \tag{12.12}$$

This is obviously zero if $m < n$ so:

$$\int_{-1}^{1} \frac{dx}{[1-x^2]^{\frac{1}{2}}} T_n(x) T_m(x) = 0 \qquad n \neq m.$$

and

$$\begin{aligned}
\int_{-1}^{1} \frac{dx}{[1-x^2]^{\frac{1}{2}}} T_n(x) T_m(x) &= \delta_{nm} \int_{-1}^{1} \frac{dx}{[1-x^2]^{\frac{1}{2}}} T_n(x) T_n(x) \\
&= \delta_{nm} \int_{-1}^{1} \frac{dx}{[1-x^2]^{\frac{1}{2}}} [(-1)^n 2^{n-1} x^n] T_n(x). \\
&= \delta_{nm} \int_{-1}^{1} \frac{dx}{[1-x^2]^{\frac{1}{2}}} [(-1)^n 2^{n-1} x^n]^2
\end{aligned} \tag{12.13}$$

Let us consider the case $m = n$. To perform the integral we make the substituition $x = \cos\theta$. Note

$$dx = -\sin\theta d\theta = -\sqrt{1-\cos^2\theta}\, d\theta = \sqrt{1-x^2}(-d\theta)$$

We need to know

$$\int_{-1}^{1} \frac{dx}{[1-x^2]^{\frac{1}{2}}} x^{2n} = \int_0^{\pi} d\theta \cos^{2n}\theta$$

Define

$$C_n = \int_0^{\pi} d\theta \cos^{2n}\theta$$

We already know

$$C_0 = \pi, \qquad C_1 = \int_0^{\pi} d\theta \cos^2\theta = \frac{\pi}{2}$$

$$
\begin{aligned}
C_n &= [\sin\theta\cos\theta]_0^\pi + (2n-1)\int_0^\pi d\theta \sin^2\theta\cos^{2n-2}\theta \\
&= (2n-1)\int_0^\pi d\theta(1-\cos^2\theta)\cos^{2n-2}\theta \\
&= (2n-1)C_{n-1} - (2n-1)C_n \qquad (12.14)
\end{aligned}
$$

$$
C_n = \frac{2n-1}{2n}C_{n-1}
$$

So that

$$
\begin{aligned}
C_n &= \frac{2n-1}{2n}\frac{2n-3}{2n-1} \\
&= \frac{(2n)!}{2^{2n}n!}\pi \qquad (12.15)
\end{aligned}
$$

$$
\begin{aligned}
\int_{-1}^1 \frac{dx}{[1-x^2]^{\frac{1}{2}}}T_n(x)T_m(x) &= \delta_{nm}[2^{n-1}]^2\int_{-1}^1 \frac{dx}{[1-x^2]^{\frac{1}{2}}}x^{2n} \\
&= \delta_{nm}\ 2^{2n-1}\frac{(2n)!}{2^{2n}n!}\pi \\
&= \delta_{nm}\ \frac{(2n)!}{2n!}\pi \qquad (12.16)
\end{aligned}
$$

To have normalised polynomial (12.4) should be replaced by

$$
T_n(x) = (-1)^n\sqrt{\frac{2n!}{(2n)!\pi}}[1-x^2]^{\frac{1}{2}}\left[\frac{d}{dx}\right]^n[1-x^2]^{n-\frac{1}{2}} \qquad (12.17)
$$

(ii)

We first note

$$
\frac{d}{dx}[1-x^2]^{n-\frac{1}{2}} = -(2n-1)x[1-x^2]^{n-1-\frac{1}{2}} \qquad (12.18)
$$

or

$$(1-x^2)\frac{d}{dx}[1-x^2]^{n-\frac{1}{2}} + (2n-1)x[1-x^2]^{n-\frac{1}{2}} = 0 \qquad (12.19)$$

and set

$$T_n' = [1-x^2]^{-\frac{1}{2}}T_n = \left[\frac{d}{dx}\right]^n [1-x^2]^{n-\frac{1}{2}}.$$

From (the 'truncated') Leibnitz,

$$\left(\frac{d}{dx}\right)^{n+1}(xf(x)) = x\left(\frac{d}{dx}\right)^{n+1} f(x) + (n+1)\left(\frac{d}{dx}\right)^n f(x).$$

and

$$\left(\frac{d}{dx}\right)^{n+1}(x^2g(x)) = x^2\left(\frac{d}{dx}\right)^{n+1} g(x) + (n+1)2x\left(\frac{d}{dx}\right)^n g(x) + (n+1)n\left(\frac{d}{dx}\right)^{n-1} g(x).$$

This leads to

$$\begin{aligned}
& \left(\frac{d}{dx}\right)^{n+1}[(1-x^2)g(x)] \\
= & \left(\frac{d}{dx}\right)^{n+1} g(x) - \left(\frac{d}{dx}\right)^{n+1}(x^2g(x)) \\
= & (1-x^2)\left(\frac{d}{dx}\right)^{n+1} g(x) - 2(n+1)x\left(\frac{d}{dx}\right)^n g(x) - n(n+1)\left(\frac{d}{dx}\right)^{n-1} g(x).
\end{aligned}$$

Applying $\left(\frac{d}{dx}\right)^{n+1}$ to (12.19) we obtain

$$
\begin{aligned}
&\left(\frac{d}{dx}\right)^{n+1}\left[(1-x^2)\frac{d}{dx}[1-x^2]^{n-\frac{1}{2}}+(2n-1)x[1-x^2]^{n-\frac{1}{2}}\right]= \\
= \;& (1-x^2)\frac{d^2}{dx^2}\left(\frac{d}{dx}\right)^n[1-x^2]^{n-\frac{1}{2}}-2(n+1)x\frac{d}{dx}\left(\frac{d}{dx}\right)^n[1-x^2]^{n-\frac{1}{2}} \\
& -n(n+1)\left(\frac{d}{dx}\right)^n[1-x^2]^{n-\frac{1}{2}} \\
& +(2n-1)x\frac{d}{dx}\left(\frac{d}{dx}\right)^n[1-x^2]^{n-\frac{1}{2}}+(2n-1)(n+1)\left(\frac{d}{dx}\right)^n[1-x^2]^{n-\frac{1}{2}} \\
= \;& (1-x^2)\frac{d^2}{dx^2}T'_n-2(n+1)x\frac{d}{dx}T'_n-n(n+1)T'_n+(2n-1)x\frac{d}{dx}T'_n+(2n-1)(n+1)T'_n \\
= \;& (1-x^2)\frac{d^2}{dx^2}T'_n-3x\frac{d}{dx}T'_n+(n^2-1)T'_n=0. \qquad (12.20)
\end{aligned}
$$

Using Leibnitz we have

$$
\begin{aligned}
\frac{d^2}{dx^2}([1-x^2]^{-\frac{1}{2}}T_n) &= [1-x^2]^{-\frac{1}{2}}\frac{d^2T_n}{dx^2}+2\frac{d}{dx}[1-x^2]^{-\frac{1}{2}}\frac{dT_n}{dx}+\frac{d^2}{dx^2}[1-x^2]^{-\frac{1}{2}}T_n \\
&= [1-x^2]^{-\frac{1}{2}}\frac{d^2T_n}{dx^2}+2x[1-x^2]^{-\frac{3}{2}}\frac{dT_n}{dx}+(1+2x^2)[1-x^2]^{-\frac{5}{2}}T_n
\end{aligned}
$$

and

$$
\frac{d}{dx}([1-x^2]^{-\frac{1}{2}}T_n)=[1-x^2]^{-\frac{1}{2}}\frac{dT_n}{dx}+x[1-x^2]^{-\frac{3}{2}}T_n
$$

Substituting these into the last line of (12.20) and multiplying by $[1-x^2]^{\frac{1}{2}}$

$$
\begin{aligned}
& (1-x^2)\left(\frac{d^2T_n}{dx^2}+2x[1-x^2]^{-1}\frac{dT_n}{dx}+(1+2x^2)[1-x^2]^{-2}T_n\right) \\
& -3x\left(\frac{dT_n}{dx}+x[1-x^2]^{-1}T_n\right)+(n^2-1)T_n=0 \\
= \;& (1-x^2)\frac{d^2T_n}{dx^2}-x\frac{dT_n}{dx}+\left(\frac{1+2x^2}{1-x^2}+\frac{-3x^2}{1-x^2}+(n^2-1)\right)T_n
\end{aligned}
$$

which easily simplifies to

$$
(1-x^2)\frac{d^2T_n}{dx^2}-x\frac{dT_n}{dx}+n^2T_n=0.
$$

(iii)

From the previous equation

$$u_0 = 1 - x^2, \qquad u_1 = -x, \qquad u_2 = n^2$$

so:

$$\begin{aligned} A(x) &= \exp\left[\int^x dx' \frac{-x'}{1-x'^2}\right] \\ &= \exp\left[\frac{1}{2}\ln(1-x^2)\right] \\ &= [1-x^2]^{\frac{1}{2}} \end{aligned}$$

and

$$B(x) = \frac{u_2}{u_0}A(x) = \frac{n^2}{[1-x^2]^{\frac{1}{2}}}$$

The resulting self-adjoint operator is

$$\hat{O} = \frac{d}{dx}\left[[1-x^2]^{\frac{1}{2}}\frac{d}{dx}\right] + \frac{n^2}{[1-x^2]^{\frac{1}{2}}}. \tag{12.21}$$

Imposing

$$\hat{O}T_n = 0$$

implies that the self-adjoint operator

$$\hat{T} = -\frac{d}{dx}\left[[1-x^2]^{\frac{1}{2}}\frac{d}{dx}\right] \tag{12.22}$$

satisfies the equation

$$\hat{T}(x)T_n(x) = \frac{n^2}{[1-x^2]^{\frac{1}{2}}}T_n(x).$$

(iv) With $x = \cos\theta$ and

$$\frac{d}{dx} = \frac{-1}{\sin\theta}\frac{d}{d\theta}$$

equation (12.3) becomes

$$\begin{aligned}
& (1-x^2)\frac{d^2T_n}{dx^2} - x\frac{dT_n}{dx} + n^2T_n \\
= \;& \sin^2\theta\left(\frac{1}{\sin\theta}\frac{d}{d\theta}\right)\frac{1}{\sin\theta}\frac{dT_n}{d\theta} + \cos\theta\frac{1}{\sin\theta}\frac{dT_n}{d\theta} + n^2T_n \\
= \;& \frac{d^2T_n}{d\theta^2} + \sin\theta\frac{-\cos\theta}{\sin^2\theta}\frac{dT_n}{d\theta} + \cos\theta\frac{1}{\sin\theta}\frac{dT_n}{d\theta} + n^2T_n \\
= \;& \frac{d^2T_n}{d\theta^2} + n^2T_n = 0 \qquad (12.23)
\end{aligned}$$

which is of Fourier type differential equation with eigenvalue $n^2$ and has the general solution

$$T_n(\cos\theta) = A\cos n\theta + B\sin n\theta$$

and we had $-1 \le x \le 1$, we must have $\pi \ge \theta \ge 0$.

What should we take for $A$ and $B$? First we note that $T_n(-x) = (-1)^nT_n(x)$ which follows from

$$T_n(-x) = [1-(-x)^2]^{\frac{1}{2}}\left[\frac{d}{-dx}\right]^n[1-(-x)^2]^{n-\frac{1}{2}} = (-1)^nT_n(x),$$

then writing

$$f_n(\phi) \equiv T_n(\cos(\frac{\pi}{2}+\phi)),$$

($-\frac{\pi}{2} \le \phi \le \frac{\pi}{2}$), we have that

$$\begin{aligned}
f_n(-\phi) &= T_n(\cos(\frac{\pi}{2}-\phi)) \\
&= T_n(-\cos(\frac{\pi}{2}+\phi)) \\
&= (-1)^nT_n(\cos(\frac{\pi}{2}+\phi)) \\
&= (-1)^nf_n(\phi).
\end{aligned}$$

Write

$$f_n(\phi) = T_n(\cos(\frac{\pi}{2} + \phi)) = A\cos n(\frac{\pi}{2} + \phi) + B\sin n(\frac{\pi}{2} + \phi)$$

and note that for $n$ odd, $\cos n(\frac{\pi}{2} + \phi)$ is an odd function in $\phi$ and $\sin n(\frac{\pi}{2} + \phi)$ is an even function in $\phi$. And for $n$ even, $\cos n(\frac{\pi}{2} + \phi)$ is an even function in $\phi$ and $\sin n(\frac{\pi}{2} + \phi)$ is an odd function in $\phi$. For consistency with $f_n(-\phi) = (-1)^n f_n(\phi)$ requires $B = 0$. The condition $T_n(1) = 1$ would require $A = 1$. So the solution is

$$T_n(\cos\theta) = \cos(n\theta). \tag{12.24}$$

We now calculate $\int_0^\pi d\theta T_m(\cos\theta)T_n(\cos\theta) = \int_0^\pi d\theta \cos n\theta \cos m\theta$. Say first $m \neq n$, then

$$\begin{aligned}
\int_0^\pi d\theta \cos m\theta \cos n\theta &= \frac{1}{2}\int_0^\pi d\theta[\cos(m+n)\theta + \cos(m-n)\theta] \\
&= \left[\frac{1}{m+n}\sin(m+n)\theta + \frac{1}{m-n}\sin(m-n)\theta\right]_0^\pi \\
&= 0.
\end{aligned}$$

Now say $m = n$. First take $n = 0$:

$$\int_0^\pi d\theta = \pi$$

and for $n > 0$

$$\int_0^\pi d\theta \cos^2 n\theta = \frac{1}{2}\int_0^\pi d\theta(\cos^2 n\theta + \sin^2 n\theta) = \frac{1}{2}\pi.$$

We used $x = \cos\theta$ so $\theta = \cos^{-1} x$ and then

$$T_n(x) = \cos(n\cos^{-1} x) \tag{12.25}$$

where

$$\int_{-1}^1 \frac{dx}{[1-x^2]^{\frac{1}{2}}} T_m(x)T_n(x) = \delta_{mn}\left\{\begin{array}{cc} \pi & n = 0 \\ \pi/2 & n > 0 \end{array}\right. \tag{12.26}$$

We can turn (12.25) into an explicit expression for $T_n(x)$. In the following keep in mind that $0 \leq x^2 \leq 1$. So we have

$$\begin{aligned} e^{i\theta} &= \cos\theta + i\sin\theta \\ &= x + i\sqrt{1-x^2} \\ &= x + \sqrt{x^2-1} \end{aligned}$$

and obviously

$$\begin{aligned} e^{-i\theta} &= \cos\theta - i\sin\theta \\ &= x - i\sqrt{1-x^2} \\ &= x - \sqrt{x^2-1} \end{aligned}$$

then

$$\begin{aligned} T_n(x) &= \cos n\theta \\ &= \frac{e^{in\theta} + e^{-in\theta}}{2} \\ &= \frac{1}{2}\left((x+\sqrt{x^2-1})^n + (x-\sqrt{x^2-1})^n\right). \end{aligned} \tag{12.27}$$

Using this, we find the first few polynomials:

$$T_0(x) = 1, \quad T_1(x) = x,$$

$$\begin{aligned} T_2(x) &= \frac{1}{2}\left((x+\sqrt{x^2-1})^2 + (x-\sqrt{x^2-1})^2\right) \\ &= \frac{1}{2}[x^2 + 2x\sqrt{x^2-1} + (x^2-1)] + \frac{1}{2}[x^2 - 2x\sqrt{x^2-1} + (x^2-1)] \\ &= x^2 + (x^2-1) \end{aligned}$$

and

$$
\begin{aligned}
T_3(x) &= \frac{1}{2}\left((x+\sqrt{x^2-1})^3+(x-\sqrt{x^2-1})^3\right) \\
&= \frac{1}{2}[x^3+3\sqrt{x^2-1}x^2+3\sqrt{x^2-1}^2x+\sqrt{x^2-1}^3] \\
+ &\ \ \frac{1}{2}[x^3-3\sqrt{x^2-1}x^2+3\sqrt{x^2-1}^2x-\sqrt{x^2-1}^3] \\
&= x^3+(x^2-1)x
\end{aligned}
$$

Note the terms involving odd powers of $\sqrt{x^2-1}$ cancel leaving a (real) polynomial. Let us consider the general case:

$$
\begin{aligned}
T_n(x) &= \frac{1}{2}\left((x+\sqrt{x^2-1})^n+(x-\sqrt{x^2-1})^n\right) \\
&= \frac{1}{2}\left(\sum_{r=0}^{n} C^n_r(x^2-1)^{\frac{r}{2}}x^{n-r}+\sum_{r=0}^{n} C^n_r(-1)^r(x^2-1)^{\frac{r}{2}}x^{n-r}\right) \\
&= \sum_{k=0}^{\lfloor\frac{n}{2}\rfloor} C^n_{2k}(x^2-1)^k x^{n-2k} \\
&= x^n\sum_{k=0}^{\lfloor\frac{n}{2}\rfloor} C^n_{2k}(1-x^{-2})^k \qquad (12.28)
\end{aligned}
$$

where $\lfloor\frac{n}{2}\rfloor$ is equal to $\frac{n}{2}$ if $n$ is even and equal to $\frac{n-1}{2}$ if $n$ is odd.

Writing it out explicitly:

$$
\begin{aligned}
& T_n(x) \\
= \ & x^n\sum_{k=0}^{\lfloor\frac{n}{2}\rfloor} C^n_{2k}(1-x^{-2})^k \\
= \ & x^n[C^n_0+C^n_2(1-x^{-2})+C^n_4(1-x^{-2})^2+C^n_6(1-x^{-2})^3+\cdots+C^n_{2\lfloor\frac{n}{2}\rfloor}(1-x^{-2})^{\lfloor\frac{n}{2}\rfloor}] \\
= \ & x^nC^n_0+ \\
+ \ & x^nC^n_2(1-x^{-2})+ \\
+ \ & x^nC^n_4(1-2x^{-2}+x^{-4})+ \\
+ \ & x^nC^n_6(1-3x^{-2}+3x^{-4}-x^{-6})+ \\
+ \ & \ldots \\
+ \ & x^nC^n_{2\lfloor\frac{n}{2}\rfloor}(1-C^{\lfloor\frac{n}{2}\rfloor}_1x^{-2}+C^{\lfloor\frac{n}{2}\rfloor}_2x^{-4}+\cdots+(-1)^{\lfloor\frac{n}{2}\rfloor-1}C^{\lfloor\frac{n}{2}\rfloor}_{\lfloor\frac{n}{2}\rfloor-1}x^{-2(\lfloor\frac{n}{2}\rfloor-1)}+(-1)^{\lfloor\frac{n}{2}\rfloor}x^{-2\lfloor\frac{n}{2}\rfloor}) \\
& \qquad (12.29)
\end{aligned}
$$

We can read off that the coefficients of each term in the power series:

$$
\begin{aligned}
&\text{coefficient of } x^n: \; C_0^n + C_2^n + C_4^n + C_6^n + C_8^n + C_{10}^n + \cdots + C_{2\lfloor \frac{n}{2} \rfloor}^n \\
&\text{coefficient of } x^{n-2}: \; -[C_2^n + 2C_4^n + 3C_6^n + 4C_8^n + 5C_{10}^n + \cdots + C_{2\lfloor \frac{n}{2} \rfloor}^n] \\
&\text{coefficient of } x^{n-4}: \; C_4^n + \frac{3 \times 2}{2} C_6^n + \frac{4 \times 3}{2} C_8^n + \frac{5 \times 4}{2} C_{10}^n + \cdots + C_{2\lfloor \frac{n}{2} \rfloor}^n \\
&\text{coefficient of } x^{n-6}: \; -[C_6^n + \frac{4 \times 3 \times 2}{3!} C_8^n + \frac{5 \times 4 \times 3}{3!} C_{10}^n + \cdots + C_{2\lfloor \frac{n}{2} \rfloor}^n]
\end{aligned}
\tag{12.30}
$$

and so on...

We dont derive forumla for these binomial coefficient summations, instead we give the explicit formula for the power series in descending powers of $x$ and demostrate it is correct via the method of proof by induction.

## 12.2 Gram-Schmidt Orthonormalisation

We include the Gram-Schmidt orthonormalisation method as an exercise. Note that since $T_n(-x) = (-1)^n T_n(x)$ that we should find that for $n$ even the terms of the polynomial will always be of even power in $x$, and for $n$ odd the terms of the polynomial will always be odd power in $x$.

We need to know

$$\int_{-1}^{1} \frac{dx}{[1 - x^2]^{\frac{1}{2}}} x^{2n} = \frac{(2n)!}{2^{2n} n!} \pi$$

and

$$\int_{-1}^{1} \frac{dx}{[1 - x^2]^{\frac{1}{2}}} x^{2n+1} = 0.$$

for $n = 0, 1, 2, \ldots$ (where we go by convention setting $0! = 1$).

Put

$$P_0 = 1 \tag{12.31}$$

$P_1 = x - a_0$

$$0 = (P_0, P_1) = \int_{-1}^{1} \frac{dx}{[1-x^2]^{\frac{1}{2}}}(x - a_0) = 0 - a_0\pi \tag{12.32}$$

implying $a_0 = 0$, so that

$$P_1 = x. \tag{12.33}$$

Put $P_2 = x^2 - a_1 P_1 - a_0 P_0$ and require

$$\begin{aligned} 0 = (P_0, P_2) &= \int_{-1}^{1} \frac{dx}{[1-x^2]^{\frac{1}{2}}} P_0(x^2 - a_1 P_1 - a_0) \\ &= \frac{\pi}{2} - a_0\pi \end{aligned}$$

and

$$\begin{aligned} 0 = (P_1, P_2) &= \int_{-1}^{1} \frac{dx}{[1-x^2]^{\frac{1}{2}}} x(x^2 - a_1 x - a_0) \\ &= -a_1 \frac{\pi}{2} \end{aligned}$$

so that

$$P_2 = x^2 - \frac{1}{2} \tag{12.34}$$

and so on...

## 12.3 Power Series Expression

We claim the power series in descending powers of $x$ is given by the formula:

$$T_n(x) = \frac{n}{2} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k \frac{(n-k-1)!}{k!(n-2k)!}(2x)^{n-2k} \qquad n > 0. \tag{12.35}$$

### 12.3.1 Recursive Relation

The proof begins by deriving a recursive relation directly as a trig identity:

$$\begin{aligned} 2\cos\theta\cos n\theta &= \frac{e^{i\theta}+e^{-i\theta}}{2}\frac{e^{in\theta}+e^{-in\theta}}{2} \\ &= \frac{e^{i(n+1)\theta}+e^{-i(n+1)\theta}}{2}+\frac{e^{i(n-1)\theta}+e^{-i(n-1)\theta}}{2} \\ &= \cos(n+1)\theta+\cos(n-1)\theta \end{aligned}$$

and so

$$\cos(n+1)\theta = 2\cos\theta\cos n\theta - \cos(n-1)\theta \tag{12.36}$$

which in terms of Chebyshev polynomials is

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x). \tag{12.37}$$

### 12.3.2 Proof by induction

We can use this recursive relation to prove (12.35) by induction.

First we assume it is true for $n-1$ and $n$ and substitute this assumption into the right hand side of the recursive relation (12.37):

$$T_{n+1}(x) = \frac{n}{2}\sum_{k=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^k\frac{(n-k-1)!}{k!(n-2k)!}(2x)^{n+1-2k} - \frac{n-1}{2}\sum_{k=0}^{\lfloor\frac{n-1}{2}\rfloor}(-1)^k\frac{(n-1-k-1)!}{k!(n-1-2k)!}(2x)^{n-1-2k} \tag{12.38}$$

and write $k = k' - 1$ in the second summation

$$\frac{n}{2}\sum_{k=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^k\frac{(n-k-1)!}{k!(n-2k)!}(2x)^{n+1-2k} - \frac{n-1}{2}\sum_{k'=1}^{\lfloor\frac{n-1}{2}\rfloor+1}(-1)^{k'-1}\frac{(n-k'-1)!}{(k'-1)!(n+1-2k)!}(2x)^{n+1-2k'}. \tag{12.39}$$

It is easy to check for $n$ even $\lfloor\frac{n-1}{2}\rfloor + 1 = \lfloor\frac{n}{2}\rfloor$ and for $n$ odd $\lfloor\frac{n-1}{2}\rfloor + 1 = \frac{n+1}{2} = \lfloor\frac{n+1}{2}\rfloor$.

We deal with the even case first:

Separating out the $k = 0$ term in the first summation andreplacing $k'$ by $k$ we obtain

$$\frac{n}{2}\frac{(n-1)!}{0!n!}(2x)^{n+1} + \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor}(-1)^k \left[\frac{n}{2}\frac{(n-k-1)!}{k!(n-2k)!} + \frac{n-1}{2}\frac{(n-k-1)!}{(k-1)!(n-2k+!)!}\right](2x)^{n+1-2k} \tag{12.40}$$

The content of the square brackets simplify:

$$\begin{aligned} \frac{1}{2}\frac{(n-k-1)!}{k!(n+1-2k)!}\{n(n+1-2k)+k(n-1)\} &= \frac{1}{2}\frac{(n-k-1)!}{k!(n+1-2k)!}\{(n+1)(n-k)\} \\ &= \frac{n+1}{2}\frac{(n-k)!}{k!(n+1-2k)!} \end{aligned} \tag{12.41}$$

and for the isolated term;

$$\frac{n}{2}\frac{(n-1)!}{0!n!}(2\cos\theta)^{n+1} = \frac{1}{2}(2\cos\theta)^{n+1} = \frac{n+1}{2}\frac{(n-0)!}{0!(n+1-0)!}(2\cos\theta)^{n+1-0}$$

and so we have

$$T_{n+1}(x) = \frac{n+1}{2}\sum_{k=0}^{\lfloor \frac{n+1}{2} \rfloor}(-1)^k \frac{(n+1-k-1)!}{k!(n+1-2k)!}(2x)^{n+1-2k}. \tag{12.42}$$

where we have used $\lfloor \frac{n+1}{2} \rfloor = \frac{n}{2} = \lfloor \frac{n}{2} \rfloor$ for $n$ even.

We now do $n$ odd:

We can go through the same steps as before, but this time there is an extra term. So from (12.39) we have

$$\begin{aligned} &\frac{n+1}{2}\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor}(-1)^k \frac{(n+1-k-1)!}{k!(n+1-2k)!}(2x)^{n+1-2k} + \left(k' = \frac{n+1}{2} \text{ in second part of (12.39)}\right) \\ = \quad & \quad \dots \quad + \frac{n-1}{2}(-1)^{\frac{n+1}{2}}\frac{(n-\frac{n+1}{2}-1)!}{(\frac{n+1}{2}-1)!(n+1-2\frac{n+1}{2})!}(2x)^{n+1-2\frac{n+1}{2}} \\ = \quad & \quad \dots \quad + \frac{n-1}{2}\frac{2}{n-1}(-1)^{\frac{n+1}{2}} \\ = \quad & \quad \dots \quad + (-1)^{\frac{n+1}{2}} \end{aligned} \tag{12.43}$$

But we get from:

$$\frac{n+1}{2}(-1)^{\frac{n+1}{2}}\frac{(n+1-\frac{n+1}{2}-1)!}{(\frac{n+1}{2})!(n+1-2\frac{n+1}{2})!}(2x)^{n+1-2\frac{n+1}{2}} = (-1)^{\frac{n+1}{2}}\frac{n+1}{2}\frac{(\frac{n-1}{2})!}{(\frac{n+1}{2})!(0)!} = (-1)^{\frac{n+1}{2}}$$

and so we have

$$T_{n+1}(x) = \frac{n+1}{2}\sum_{k=0}^{\lfloor\frac{n+1}{2}\rfloor}(-1)^k\frac{(n+1-k-1)!}{k!(n+1-2k)!}(2x)^{n+1-2k}.$$

So we have obtained the correct formula, i.e. (12.35) with $n \mapsto n+1$, for both $n$ even and $n$ odd.

Now we can argue that if it works for $n = 1$ and for $n = 2$ then it works for $n = 3$. We then know it works for $n = 2$ and for $n = 3$ therefore it works for $n = 4$, and so on...

So for $n = 1$:

$$\frac{1}{2}\sum_{k=0}^{0}(-1)^0\frac{(0-k)!}{0!(1-2\times k)!}(2x)^1 = \frac{1}{2}\frac{0!}{0!1!}2x = x = T_1(x)$$

and for $n = 2$:

$$\frac{2}{2}\sum_{k=0}^{1}(-1)^k\frac{(1-k)!}{k!(2-2k)!}(2x)^{2-2k} = 2x^2 - 1 = T_2(x).$$

We have then derived the power series expansion for $\cos n\theta$ in terms of $\cos\theta$:

$$\cos n\theta = \frac{n}{2}\sum_{k=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^k\frac{(n-k-1)!}{k!(n-2k)!}(2\cos\theta)^{n-2k} \qquad n > 0. \tag{12.44}$$

### 12.3.3 Binomial coefficient summation identities

From this result we have inadvertently derived the binomial coefficient summation identities (see (12.30)):

$$
\begin{aligned}
C_0^n + C_2^n + C_4^n + C_6^n + C_8^n + C_{10}^n + \cdots + C_{2\lfloor\frac{n}{2}\rfloor}^n &= 2^{n-1} \\
C_2^n + 2C_4^n + 3C_6^n + 4C_8^n + 5C_{10}^n + \cdots + C_{2\lfloor\frac{n}{2}\rfloor}^n &= n2^{n-3} \\
C_4^n + \frac{3\times 2}{2}C_6^n + \frac{4\times 3}{2}C_8^n + \frac{5\times 4}{2}C_{10}^n + \cdots + C_{2\lfloor\frac{n}{2}\rfloor}^n &= \frac{n(n-3)}{2}2^{n-5} \\
C_6^n + \frac{4\times 3\times 2}{3!}C_8^n + \frac{5\times 4\times 3}{3!}C_{10}^n + \cdots + C_{2\lfloor\frac{n}{2}\rfloor}^n &= \frac{n(n-3)(n-5)}{3!}2^{n-7}
\end{aligned}
\tag{12.45}
$$

and so on...

## 12.4 Table of Chebyshev Polynomials

$$
\begin{aligned}
T_0(x) &= 1 \\
T_1(x) &= x \\
T_2(x) &= 2x^2 - 1 \\
T_3(x) &= 4x^3 - 3x \\
T_4(x) &= 8x^4 - 8x^2 + 1 \\
T_5(x) &= 16x^5 - 20x^3 + 5x \\
T_6(x) &= 32x^6 - 48x^4 + 18x^2 - 1
\end{aligned}
\tag{12.46}
$$

# Chapter 13

# Orthogonal Curvilinear Coordinates

When a problem has symmetry the analysis is greatly simplified by a coordinate system which respects the symmetry. Rotational symmetry about an axis is best described by cylindrical polar coordinates, where the absence of dependence on the polar angle in the description corresponds to the symmetry. Spherical symmetry is best described by spherical polar coordinates, where the absence of dependence on the two polar angles amounts to the symmetry.

Curvilnear coordinates are a coordinate system for Euclidean space in which the coordinate lines may be curved. We have already met such coordinates - cylindrical and spherical polar coordinates.

We will use Guass's theroem and Stoke's theorem to find formula for the Divergence and Curl respectively in orthogonal curvilinear coordinates. We have already derived formula for the Gradient in the main text,combining this with formula for the Divergence we will obtain a formula for the Laplacian of a scalar field.

You first need to construct this picture for your coordinate system. The crucial and central equation is:

$$\mathbf{dr} = h_u du \hat{\mathbf{u}} + h_v dv \hat{\mathbf{v}} + h_w \hat{\mathbf{w}}$$

which can be read off from the picture.

'Curvilinear ccordinates' are coordinate systems which are locally orthogonal, but can vary their orientation as we move around in space. The natural examples are cylindrical polar coordinates $(\rho, \phi, z)$ and spherical polar coordinates $(r, \theta, \phi)$.

(i) Cylindrical polar coordinates

so $h_\rho = 1$, $h_\phi = \rho$ and $h_z = 1$.

(ii) Spherical polar coordinates

so $h_r = 1$, $h_\theta = r$ and $h_\phi = r\sin\theta$.

Perhaps the simplest applicationof this theory is to volume integrals. The volume of the cube is simply:

$$dv = h_u h_v h_w du dv dw$$

and consequently:

$$dV = r dr d\phi dz \qquad \text{and} \qquad dV = r^2 dr \sin\theta d\theta d\phi$$

for cylindrical and polar coordinates respectively.

**Example: Evaluate:**

$$I(a) = \int_{V(a)} dx dy dz \ln\left[x^2 + y^2 + z^2\right]^{\frac{1}{2}}$$

where $V(a)$ is a sphere of radius $a$.

Use spherical polar coordinates:

$$\begin{aligned} I(a) &= \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \int_0^a dr r^2 \ln r = 4\pi \left( \left[ \frac{r^3}{3} \ln r \right]_0^a - \int_0^a dr \frac{r^3}{3}\frac{1}{r} \right) \\ &= 4\pi \left[ \frac{a^3 \ln a}{3} - \frac{a^3}{9} \right] = \frac{4\pi}{9} a^3 \left[\ln a^3 - 1\right] \end{aligned} \tag{13.1}$$

## 13.1 The Grad of a Scalar

$\nabla V$ defined by $\delta V - \delta\mathbf{r} \cdot \nabla V$. For $u \mapsto u + \delta u$,

$$\delta V = \delta u \frac{\partial V}{\partial u} = h_u \delta u \hat{\mathbf{u}} \cdot \nabla V$$

and so:

$$\nabla V = \frac{1}{h_u}\frac{\partial V}{\partial u}\hat{\mathbf{u}} + \frac{1}{h_v}\frac{\partial V}{\partial v}\hat{\mathbf{v}} + \frac{1}{h_w}\frac{\partial V}{\partial w}\hat{\mathbf{w}}.$$

## 13.2 The Divergence

We can use the Gauss's Divergence theorem to find a formula for the divergence.

$$\nabla \cdot \vec{v}\,(q_1, q_2, q_3) = \lim_{dV \to 0} \frac{\int \vec{v} \cdot d\vec{S}}{\int dV} \tag{13.2}$$

with differencial volume

$$dV = h_1 h_2 h_3 dq_1 dq_2 dq_3.$$

Define

$$v_1 = \vec{v} \cdot \vec{e}_1, \quad v_2 = \vec{v} \cdot \vec{e}_2, \quad v_1 = \vec{v} \cdot \vec{e}_3.$$

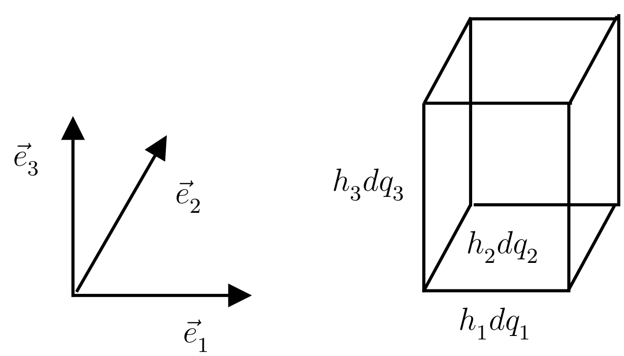



Figure 13.1: The gradient of $\vec{v}$.

The area integral for the two faces $q_1 = Const.$ is given by

$$\left[v_1 h_2 h_3 + \frac{\partial}{\partial q_1}(v_1 h_2 h_3) dq_1\right] dq_2 dq_3 - v_1 h_2 h_3 dq_2 dq_3 = \frac{\partial}{\partial q_1}(v_1 h_2 h_3) dq_1 dq_2 dq_3. \tag{13.3}$$

Adding in similar results for the other two pair of surfaces, we obtain

$$\int \vec{v}\,(q_1, q_2, q_3) \cdot d\vec{S} = \left[\frac{\partial(v_1 h_2 h_3)}{\partial q_1} + \frac{\partial(v_2 h_1 h_3)}{\partial q_2} + \frac{\partial(v_3 h_1 h_2)}{\partial q_3}\right] dq_1 dq_2 dq_3. \tag{13.4}$$

And division by the diffrential volume (13.2) yields

$$\nabla \cdot \vec{v}\,(q_1, q_2, q_3) = \frac{1}{h_1 h_2 h_3}\left[\frac{\partial(v_1 h_2 h_3)}{\partial q_1} + \frac{\partial(v_2 h_1 h_3)}{\partial q_2} + \frac{\partial(v_3 h_1 h_2)}{\partial q_3}\right] \tag{13.5}$$

## 13.3 Laplacian of a Scalar

Combining (??) and (13.5) we obtain the formula for the Laplacian of a scalar field,

$$\nabla^2\phi(q_1, q_2, q_3) = \frac{1}{h_1 h_2 h_3}\left[\frac{\partial}{\partial q_1}\left(\frac{h_2 h_3}{h_1}\frac{\partial\phi}{\partial q_1}\right) + \frac{\partial}{\partial q_2}\left(\frac{h_1 h_3}{h_2}\frac{\partial\phi}{\partial q_2}\right) + \frac{\partial\phi}{\partial q_3}\left(\frac{h_1 h_2}{h_3}\frac{\partial\phi}{\partial q_3}\right)\right] \tag{13.6}$$

## 13.4 The Curl

Using Stoke's theorem

$$\int \nabla\times\vec{v}\cdot d\vec{S} = \oint_C \vec{v}\cdot d\vec{l}$$

in differential form we calculate the componet $\vec{e}_1\cdot\nabla\times\vec{v}$ from

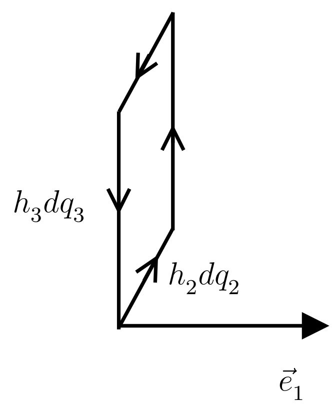



Figure 13.2: The $\vec{e}_1$ component of the Curl of an infintesimal loop.

$$\begin{aligned}\vec{e}_1\cdot\nabla\times\vec{v}\;dq_2dq_3h_2h_3 &= \left(\left[h_3v_3 + \frac{\partial}{\partial q_2}(h_3v_3)dq_2\right] - h_3v_3\right)dq_3 \\ &\quad - \left(\left[h_2v_2 + \frac{\partial}{\partial q_3}(h_2v_2)dq_3\right] - h_2v_2\right)dq_2 \end{aligned} \tag{13.7}$$

and so

$$\vec{e}_1 \cdot \nabla \times \vec{v} = \frac{1}{h_2 h_3} \left[ \frac{\partial}{\partial q_2}(h_3 v_3) - \frac{\partial}{\partial q_3}(h_2 v_2) \right] \tag{13.8}$$

Similar results for the other two rectangles, those orthogonal to $\vec{e}_2$ and $\vec{e}_3$, we obtain

$$\begin{aligned} \nabla \times \vec{v} \;\; = \;\; & \frac{1}{h_2 h_3} \left[ \frac{\partial}{\partial q_2}(h_3 v_3) - \frac{\partial}{\partial q_3}(h_2 v_2) \right] \vec{e}_1 \\ & + \frac{1}{h_1 h_3} \left[ \frac{\partial}{\partial q_3}(h_1 v_1) - \frac{\partial}{\partial q_1}(h_3 v_3) \right] \vec{e}_2 \\ & + \frac{1}{h_1 h_2} \left[ \frac{\partial}{\partial q_1}(h_3 v_3) - \frac{\partial}{\partial q_3}(h_1 v_1) \right] \vec{e}_3 \end{aligned} \tag{13.9}$$

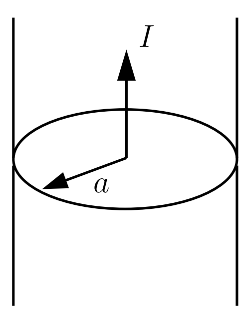
which is compactly written as

$$\begin{aligned} \nabla \times \vec{v} \;\; &= \;\; \nabla \times (v_1 \vec{e}_1 + v_2 \vec{e}_2 + v_3 \vec{e}_3) \\ &= \;\; \frac{1}{h_1 h_2 h_3} \begin{vmatrix} \vec{e}_1 h_1 & \vec{e}_2 h_2 & \vec{e}_3 h_3 \\ \dfrac{\partial}{\partial q_1} & \dfrac{\partial}{\partial q_2} & \dfrac{\partial}{\partial q_3} \\ h_1 v_1 & h_2 v_2 & h_3 v_3 \end{vmatrix} . \end{aligned} \tag{13.10}$$

### 13.4.1 Example:

A wire of radius $a$, carries a uniform current, $I$, find the resulting magnetic field distribution.

This is a cylindrical problem




$$\nabla \times \mathbf{B} = \mu_0 J$$

with $\mathbf{J} = \frac{I}{\pi a^2}\hat{z}$.

Method (i): Guess that $\mathbf{B} = B(\rho)\phi$ and use Stoke's theorem

$$\int_S \mathbf{dS} \cdot \nabla \times \mathbf{B} = \int_C \mathbf{dl} \cdot \mathbf{B}$$

$$\begin{aligned} 2\pi B(\rho) &= \frac{\pi\rho^2}{\pi a^2}\mu_0 I \quad \rho < a \\ &\phantom{=} \mu_0 I \qquad \rho > a \end{aligned}$$

so $B(\rho) = \frac{\mu_0 I}{2\pi}\frac{\rho}{a^2}$ for $\rho < a$ and $B(\rho) = \frac{\mu_0 I}{2\pi}\frac{1}{\rho}$ for $\rho > a$.

Method (ii): Use 'curvilinear coordinates'

$$\begin{aligned} \nabla \times \mathbf{B} &= \nabla \times (B_\rho \vec{\rho} + B_\phi \vec{\phi} + B_z \vec{z}) \\ &= \frac{1}{\rho}\begin{vmatrix} \vec{\rho} & \vec{\phi}\rho & \vec{z} \\ \frac{\partial}{\partial \rho} & \frac{\partial}{\partial \phi} & \frac{\partial}{\partial z} \\ B_\rho & \rho B_\phi & B_z \end{vmatrix} \\ &= \left[\frac{1}{\rho}\frac{\partial B_z}{\partial \phi} - \frac{\partial B_\phi}{\partial z}\right]\vec{\rho} \\ &+ \left[\frac{\partial B_\rho}{\partial z} - \frac{\partial B_z}{\partial \rho}\right]\vec{\phi} \\ &+ \left[\frac{1}{\rho}\frac{\partial}{\partial \rho}(\rho B_\phi) - \frac{1}{\rho}\frac{\partial B_\rho}{\partial \phi}\right]\vec{z} \end{aligned} \tag{13.11}$$

so

$$\begin{aligned} \frac{1}{\rho}\frac{\partial}{\partial \rho}(\rho B_\phi) &= \frac{\mu_0 I}{\pi a^2} \qquad \rho < a \\ &= 0 \qquad \rho > a \end{aligned}$$

Integrating once gives $\rho B(\rho) = \frac{\mu_0 I}{\pi a^2}\frac{\rho^2}{2}$ for $\rho < a$ and $\rho B(\rho) = \frac{\mu_0 I}{\pi a^2}\frac{a^2}{2}$ for $\rho > a$ as before.

### 13.4.2 Example:

A sphere of radius $a$, carries a uniform charge, $Q$, find the electric field distribution.

This problemis a spherical problem:

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$$

with $\rho = \frac{3Q}{4\pi a^3}$.

Method (i): Guess that $\mathbf{E}(\mathbf{r}) = E(r)\hat{\mathbf{r}}$ and then use Gauss's theorem

$$\int_V dV \nabla \cdot \mathbf{E} = \int_S \mathbf{dS} \cdot \mathbf{E}$$

$$4\pi r^2 E(r) = \frac{3}{4\pi a^3}\frac{4\pi r^3}{3}\frac{Q}{\epsilon_0} \qquad r < a$$

$$\frac{Q}{\epsilon_0} \qquad r > a$$

Method (ii): Use 'curvilinear coordinates' (13.5) with $h_r = 1$ $h_\theta = r$ $h_\phi = r\sin\theta$:

$$\begin{aligned} \nabla \cdot \mathbf{E} &= \frac{1}{r^2 \sin\theta}\left[\frac{\partial(r^2 \sin\theta E_r)}{\partial r} + \frac{\partial(r\sin\theta E_\theta)}{\partial \theta} + \frac{\partial(rE_\phi)}{\partial \phi}\right] \\ &= \frac{3Q}{4\pi a^3 \epsilon_0} \qquad r < a \end{aligned} \tag{13.12}$$

and $= 0$ for $r > a$. Integrating once gives $r^2 E(r) = \frac{3Q}{4\pi a^3 \epsilon_0}\frac{r^3}{3}$ for $r < a$ and $r^2 E(r) = \frac{3Q}{4\pi a^3}\frac{a^3}{3}$ for $r > a$, as before.

### 13.4.3 Change of Coordinates

The obvious question of 'How do you know whether a particular coordinate system is locally orthogonal?' emerges. Everything can be found from changes of coordinate systems combined with:

$$\mathbf{dr} = h_u du \hat{\mathbf{u}} + h_v dv \hat{\mathbf{v}} + h_w dw \hat{\mathbf{w}}$$

(1) Cylindrical, $x = \rho\cos\phi$, $y = \rho\sin\phi$ and $z = z$.

$$
\begin{aligned}
\mathbf{dr} &= dx\hat{\mathbf{x}} + dy\hat{\mathbf{y}} + dz\hat{\mathbf{z}} \\
&= (d\rho\cos\phi - d\phi\sin\phi\rho)\hat{\mathbf{x}} \ + (d\rho\sin\phi + d\phi\cos\phi\rho)\hat{\mathbf{y}} + dz\hat{\mathbf{z}} \\
&= d\rho(\cos\phi\hat{\mathbf{x}} + \sin\phi\hat{\mathbf{y}}) + \rho d\phi(-\sin\phi\hat{\mathbf{x}} + \cos\phi\hat{\mathbf{y}}) + dz\hat{\mathbf{z}} \qquad (13.13)
\end{aligned}
$$

and so $\rho = \cos\phi\hat{\mathbf{x}} + \sin\phi\hat{\mathbf{y}}$, $\phi = -\sin\phi\hat{\mathbf{x}} + \cos\phi\hat{\mathbf{y}}$ and $\rho\cdot\phi = 0$. Also, $h_\rho = 1$, $h_\phi = \rho$ and $h_z = 1$, looking at the normalisation.

(2) Spherical, $\rho = r\sin\theta$, $z = r\cos\theta$ and $\phi = \phi$.

$$
\begin{aligned}
\mathbf{dr} &= d\rho\rho + dz\hat{\mathbf{z}} + \rho d\phi\phi \\
&= (dr\sin\theta + d\theta\cos\theta r)\rho + (dr\cos\theta - d\theta\sin\theta r)\hat{\mathbf{z}} + r\sin\theta d\phi\phi \\
&= dr(\sin\theta\rho + \cos\theta\hat{\mathbf{z}}) + rd\theta(\cos\theta\rho - \sin\theta\hat{\mathbf{z}}) + r\sin\theta d\phi\phi \qquad (13.14)
\end{aligned}
$$

so $\hat{\mathbf{r}} = \sin\theta\rho + \cos\theta\hat{\mathbf{z}}$, $\theta = \cos\theta\rho - \sin\theta\hat{\mathbf{z}}$ and $\hat{\mathbf{r}}\cdot\theta = 0$. Also, $h_r = 1$, $h_\theta = r$ and $h_\phi = r\sin\theta$.

**Example:**

Parabolic coordinates: Show curvilinearity and find $\nabla^2$.

$u = r + z$, $v = r - z$ and $\phi = \phi$ are parabolic coordinates. We will start from cylindrical and transform to parabolic: $\rho = \sqrt{(uv)}$, $z = \frac{u-v}{2}$ and $\phi = \phi$.

$$
\begin{aligned}
\mathbf{dr} &= d\rho\rho + dz\hat{\mathbf{z}} + \rho d\phi\phi \\
&= \left[du\left(\frac{v}{u}\right)^{\frac{1}{2}}\frac{1}{2} + dv\left(\frac{u}{v}\right)^{\frac{1}{2}}\frac{1}{2}\right]\rho + \frac{du - dv}{2}\hat{\mathbf{z}} + \sqrt{(uv)}d\phi\phi \\
&= \frac{du}{2}\left[\hat{\mathbf{z}} + \left(\frac{v}{u}\right)^{\frac{1}{2}}\rho\right] + \frac{dv}{2}\left[-\hat{\mathbf{z}} + \left(\frac{u}{v}\right)^{\frac{1}{2}}\rho\right] + \sqrt{(uv)}d\phi\phi \qquad (13.15)
\end{aligned}
$$

so $\hat{\mathbf{u}} = \frac{\sqrt{u}\hat{\mathbf{z}} + \sqrt{v}\rho}{\sqrt{(u+v)}}$, $\hat{\mathbf{v}} = \frac{-\sqrt{v}\hat{\mathbf{z}} + \sqrt{u}\rho}{\sqrt{(u+v)}}$ and $\hat{\mathbf{u}}\cdot\hat{\mathbf{v}} = 0$. The scale factors are $h_u = \frac{1}{2}\frac{\sqrt{(u+v)}}{\sqrt{u}}$, $h_v = \frac{1}{2}\frac{\sqrt{(u+v)}}{\sqrt{v}}$ and $h_\phi = \sqrt{(uv)}$.

The Laplacian is:

$$
\begin{aligned}
\nabla^2 &= \frac{1}{h_1 h_2 h_3}\left[\frac{\partial}{\partial q_1}\left(\frac{h_2 h_3}{h_1}\frac{\partial}{\partial q_1}\right)+\frac{\partial}{\partial q_2}\left(\frac{h_1 h_3}{h_2}\frac{\partial}{\partial q_2}\right)+\frac{\partial}{\partial q_3}\left(\frac{h_1 h_2}{h_3}\frac{\partial}{\partial q_3}\right)\right] \\
&= \frac{4}{u+v}\left[\frac{\partial}{\partial u}u\frac{\partial}{\partial u}+\frac{\partial}{\partial v}v\frac{\partial}{\partial v}+\frac{u+v}{4uv}\frac{\partial^2}{\partial \phi^2}\right]. \qquad (13.16)
\end{aligned}
$$

# Chapter 14

# Quantum Mechanics

This section of the course is designed to support the quantum mechanics course with some underlying mathematics.

We will be interested in:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(|\mathbf{r}|) \tag{14.1}$$

subject to the commutation relations $[\mathbf{r}, \hat{\mathbf{p}}] = i\hbar\mathbf{I}$, where $\hat{\mathbf{p}}$ is the momentum operator and $\mathbf{r}$ is the position of the particle. We will work with the real-space wavefunction, $\psi(\mathbf{r})$. In this case the momentum operator is $\hat{\mathbf{p}} = -i\nabla$, which ensures thath the commutation relations are satisfied.

The Hamiltonian operator is then

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(|\mathbf{r}|) \tag{14.2}$$

which, with a uniform weight function and an inner product

$$(\psi_1, \psi_2) = \int_V d\mathbf{r}\psi_1^*(\mathbf{r})\psi_2(\mathbf{r}) \tag{14.3}$$

form a Sturm-Liouville type of problem. We are looking for solutions to

$$\hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r}). \tag{14.4}$$

We will pay special attention to

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}k|\mathbf{r}| \tag{14.5}$$

the simple harmonic oscillator in one and three dimensions, and

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{|\mathbf{r}|} \tag{14.6}$$

the Hydrogen atom.

## 14.1 Scaling

The first thing to do is always to scale away irrelevant parameters, i.e. choose your units very carefully.

For the current problem we can independently scale the vector, $\mathbf{r}$, and the energy, $E$.

$$\mathbf{r} \mapsto \alpha\mathbf{x}$$
$$E \mapsto \beta\epsilon$$

and the gradient operator becomes:

$$\nabla \equiv \frac{\partial}{\partial\mathbf{r}} = \left[\frac{\partial\mathbf{x}}{\partial\mathbf{r}}\right]\frac{\partial}{\partial\mathbf{x}} = \frac{1}{\alpha}\frac{\partial}{\partial\mathbf{x}}$$

so:

$$\hat{H} - E = -\frac{\hbar^2}{2m}\nabla^2 + V(|\mathbf{r}|) - E$$

becomes

$$\hat{H} - E = -\frac{\hbar^2}{2m\alpha^2}\nabla^2_{\mathbf{x}} + V(\alpha|\mathbf{x}|) - \beta\epsilon$$

and we are free to choose $\alpha$ and $\beta$ to make thisnew Hamiltonian ‘simple’.

### 14.1.1 Example: Harmonic oscillator

(i) For the harmonic oscillator $V(|\mathbf{r}|) = \frac{1}{2}k|\mathbf{r}|^2$

$$\hat{H} - E = -\frac{\hbar^2}{2m\alpha^2}\nabla_{\mathbf{x}}^2 + \frac{1}{2}k\alpha^2|\mathbf{x}|^2 - \beta\epsilon$$

we can choose $\alpha$ and $\beta$ to make all three coefficients the 'same':

$$\frac{\hbar^2}{m\alpha^2} = k\alpha^2 = \beta$$

is the usual choice, and then

$$\alpha = \left[\frac{\hbar^2}{mk}\right]^{\frac{1}{4}}$$
$$\beta = \left[\frac{k}{m}\right]^{\frac{1}{2}}\hbar$$

and the rescaled problem becomes

$$\frac{1}{\beta}\left[\hat{H} - E\right] = -\frac{1}{2}\nabla_{\mathbf{x}}^2 + \frac{1}{2}|\mathbf{x}|^2 - \epsilon$$

### 14.1.2 Example: The hydrogen atom

(ii) For the hydrogen atom $V(|\mathbf{r}|) = -\dfrac{e^2}{|\mathbf{r}|}$

$$\hat{H} - E = -\frac{\hbar^2}{2m\alpha^2}\nabla_{\mathbf{x}}^2 - \frac{e^2}{\alpha|\mathbf{x}|} - \beta\epsilon$$

we can choose $\alpha$ and $\beta$ to make all three coefficients the 'equal':

$$\frac{\hbar^2}{m\alpha^2} = \frac{e^2}{\alpha} = 2\beta$$

and so

$$\alpha = \frac{\hbar^2}{me^2}$$

$$\beta = \frac{me^4}{2\hbar^2}$$

and the rescaled problem becomes:

$$\frac{1}{\beta}\left[\hat{H} - E\right] = -\nabla^2_{\mathbf{x}} - 2\frac{1}{|\mathbf{x}|} - \epsilon.$$

Note: the inner product changes under rescalling!

# Chapter 15

# Separation of Variables

One has an equation of the form

$$\hat{O}[x_1, x_2, \ldots, x_n]\psi(x_1, x_2, \ldots, x_n) = 0. \tag{15.1}$$

One assumes that

$$\psi(x_1, x_2, \ldots, x_n) = \psi(x_1)\tilde{\psi}(x_2, \ldots, x_n)$$

and then the equation is separable if

$$\hat{O}[x_1, x_2, \ldots, x_n]\psi(x_1, x_2, \ldots, x_n) = 0. \tag{15.2}$$

## 15.1 Separtion of Variables and the 6 Sturm-Liouville Problems

Legandre

Chebyshev

Bessel

Laguerre

Simple harmonic oscillator

Hermite

## 15.2 Example (i): Simple Harmonic Oscillator

Simple harmonic oscillator in three dimensions:

$$\hat{H}_3(\mathbf{x}) = \hat{H}_1(x_1) + \hat{H}_1(x_2) + \hat{H}_1(x_3) \tag{15.3}$$

where

$$\hat{H}_1(x_i) = -\frac{1}{2}\frac{\partial^2}{\partial x_i^2} + \frac{1}{2}x_i^2 \tag{15.4}$$

The equation to solve is

$$\hat{H}_3(\mathbf{x})\psi(\mathbf{x}) \equiv \left[\hat{H}_1(x_1) + \hat{H}_1(x_2) + \hat{H}_1(x_3)\right]\psi(\mathbf{x}) = \epsilon\psi(\mathbf{x}) \tag{15.5}$$

We write $\psi(\mathbf{x})$ as the product of two functions one of which only depends on one of the coordinates,say the $x_1$ coordinate. Substituting this into (15.5) gives

$$\begin{aligned} & \left[\tilde{\psi}(x_2,x_3)\hat{H}_1(x_1)\psi_1(x_1) + \psi_1(x_1)\hat{H}_1(x_2)\tilde{\psi}(x_2,x_3) + \psi_1(x_1)\hat{H}_1(x_3)\tilde{\psi}(x_2,x_3)\right] \\ = \quad & \epsilon\psi_1(x_1)\tilde{\psi}(x_2,x_3) \end{aligned} \tag{15.6}$$

Dividing by $\psi_1(x_1)\tilde{\psi}(x_2,x_3)$ and rearranging we can write

$$\frac{1}{\tilde{\psi}(x_2,x_3)}\hat{H}_1(x_2)\tilde{\psi}(x_2,x_3) + \frac{1}{\tilde{\psi}(x_2,x_3)}\hat{H}_1(x_3)\tilde{\psi}(x_2,x_3) = \epsilon - \frac{1}{\psi_1(x_1)}\hat{H}_1(x_1)\psi_1(x_1) \tag{15.7}$$

As the RHS depends only on $x_1$ while the LHS only depends on $x_2$ and $x_3$, the RHS must equal a constant, say $\epsilon - \epsilon_1$, resulting in the ODE

$$\hat{H}_1(x_1)\psi_1(x_1) = \left[-\frac{1}{2}\frac{d^2}{dx_1^2} + \frac{1}{2}x_1^2\right]\psi_1(x_1) = \epsilon_1\psi_1(x_1)$$

where we have written the partial derivative as a total derivative as they are equivalent because the function $\psi_1$ is a function of $x_1$ alone. Equation (15.7) then becomes

$$\hat{H}_1(x_2)\tilde{\psi}(x_2,x_3) + \hat{H}_1(x_3)\tilde{\psi}(x_2,x_3) = (\epsilon - \epsilon_1)\tilde{\psi}(x_2,x_3). \tag{15.8}$$

Repeating the process, we write $\tilde{\psi}(x_2, x_3) = \psi_2(x_2)\psi_3(x_3)$, substitute it into (15.8), dividing by $\psi_2(x_2)\psi_3(x_3)$, and rearanging

$$\frac{1}{\psi_3(x_3)}\hat{H}_1(x_3)\psi_3(x_3) = (\epsilon - \epsilon_1) - \frac{1}{\psi_2(x_2)}\hat{H}_1(x_2)\psi_2(x_2)$$

Again, as the RHS only depends on $x_2$ while the LHS only depends on $x_3$ so we equate the RHS to a constant, say $\epsilon - \epsilon_1 - \epsilon_2$, then we obtain

$$\hat{H}_1(x_2)\psi_2(x_2) = \left[-\frac{1}{2}\frac{d^2}{dx_2^2} + \frac{1}{2}x_2^2\right]\psi_2(x_2) = \epsilon_2\psi_2(x_2)$$

and

$$\hat{H}_1(x_3)\psi_3(x_3) = \left[-\frac{1}{2}\frac{d^2}{dx_3^2} + \frac{1}{2}x_3^2\right]\psi_3(x_3) = (\epsilon - \epsilon_1 - \epsilon_2)\psi_3(x_3)$$

Calling $\epsilon_3 = \epsilon - \epsilon_1 - \epsilon_2$ we have in summary:

$$\epsilon = \epsilon_1 + \epsilon_2 + \epsilon_3$$

$\psi(\mathbf{x}) = \psi_1(x_1)\psi_2(x_2)\psi_3(x_3)$ and

$$\left[-\frac{1}{2}\frac{d^2}{dx_i^2} + \frac{1}{2}x_i^2\right]\psi_i(x_i) = \epsilon_i\psi_i(x)$$

for $i = 1, 2, 3$.

We see that the assumed product form of the solution is valid because it works.

## 15.3 Example (ii): Rotational Invariance: Sphererical Coordinates

$$\hat{H}(\mathbf{x}) = -\nabla_{\mathbf{x}}^2 + V(|\mathbf{x}|) \equiv -\nabla_{\mathbf{x}}^2 + V(x) \tag{15.9}$$

and from the curvilinear coordinates section

$$\nabla_{\mathbf{x}}^2 = \frac{1}{x^2}\frac{\partial}{\partial x}\left[x^2\frac{\partial}{\partial x}\right] + \frac{1}{x^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\right] + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right) \tag{15.10}$$

we wish to solve the problem

$$\hat{H}(\mathbf{x})\psi(x,\theta,\phi) = \left[-\nabla^2_{\mathbf{x}} + V(x)\right]\psi(x,\theta,\phi) = \epsilon\psi(x,\theta,\phi) \tag{15.11}$$

and

$$\psi(\mathbf{x}) = \psi_x(x)\psi_\theta(\theta)\psi_\phi(\phi) \tag{15.12}$$

leads to the one-dimensional problems:

$$-\frac{\partial^2\psi_\phi}{\partial\phi^2} = m^2\psi_\phi \tag{15.13}$$

$$\left(-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\right] + \frac{m^2}{\sin^2\theta}\psi_\theta\right) = l(l+1)\psi_\theta \tag{15.14}$$

$$\left(-\frac{1}{x^2}\left[x^2\frac{\partial}{\partial x}\right] + \frac{l(l+1)}{x^2} + V(x)\right)\psi_x = \epsilon\psi_x$$

and finally for harmonic oscillator and hydrogen atom respectively:

### 15.3.1 Harmonic oscillator

$$\left(-\frac{1}{2x^2}\left[x^2\frac{\partial}{\partial x}\right] + \frac{l(l+1)}{2x^2} + \frac{x^2}{2}\right)\psi_x = \epsilon\psi_x \tag{15.15}$$

### 15.3.2 Hydrogen atom

$$\left(-\frac{1}{x^2}\left[x^2\frac{\partial}{\partial x}\right] + \frac{l(l+1)}{x^2} + \frac{2}{x}\right)\psi_x = \epsilon\psi_x \tag{15.16}$$

## 15.4 Example (iii): Hydrogen Atom: Parabolic Coordinates

from the curvilinear coordinates section:

$$\nabla^2_{\mathbf{x}} = \frac{4}{u+v}\left(\frac{\partial}{\partial u}\left[u\frac{\partial}{\partial u}\right] + \frac{\partial}{\partial v}\left[\frac{\partial}{\partial v}\right] + \frac{u+v}{4uv}\frac{\partial^2}{\partial \phi^2}\right)$$

and $x = \frac{1}{2}(u+v)$ so:

$$V = -\frac{4}{u+v}$$

and miraculously, the equation separates!

$$\psi(x) = \psi_u(u)\psi_v(v)\psi_\phi(\phi)$$

with

$$-\frac{d^2\psi_\phi}{d\phi^2} = m^2\psi_\phi \tag{15.17}$$

$$\left(-\frac{\partial}{\partial u}\left[u\frac{\partial}{\partial u}\right] + \frac{m^2}{4u} - \frac{1}{2} - \frac{u\epsilon}{2}\right)\psi_u = \alpha\psi_u \tag{15.18}$$

$$\left(-\frac{\partial}{\partial v}\left[v\frac{\partial}{\partial v}\right] + \frac{m^2}{4v} - \frac{1}{2} - \frac{v\epsilon}{2}\right)\psi_v = -\alpha\psi_v \tag{15.19}$$

We are led to six Sturm-Lioville type problems.

## 15.5 Fourier Series

One of these problems we have encountered previously:

$$H = -\frac{d^2}{d\phi^2}$$

in the variational estimates section. In that case we had openconditions, but in this quantum mechanical context we have perio0dic boundary conditions: The angle $\phi$ is a real *physical* angle and so $\phi = 0$ *corresponds* to $\phi = 2\pi$. We require to generate solutions to:

$$-\frac{d^2\psi}{d\phi^2}(\phi) = m^2\psi(\phi)$$

subject to the boundary conditions that:

$$\psi(\phi + 2\pi) = \psi(\phi).$$

Obviously, 'sine's and cosine's will do, but it is much more effective to use a *complex* fourier series:

$$\psi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

where the boundary condition requires that:

$$\psi_m(\phi + 2\pi) = \frac{1}{\sqrt{2\pi}} e^{im(\phi+2\pi)} = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

and hence that $e^{2\pi im} = 1$ and $m$ is an integer.

The associated inner-product is:

$$(\psi, \psi') = \int_0^{2\pi} d\phi \psi^*(\phi)\psi(\phi)$$

and our choice of wavefunctions provides:

$$(\psi_n, \psi_{n'}) = \int_0^{2\pi} \frac{d\phi}{2\pi} e^{i(n'-n)\phi} = \delta_{n,n'}$$

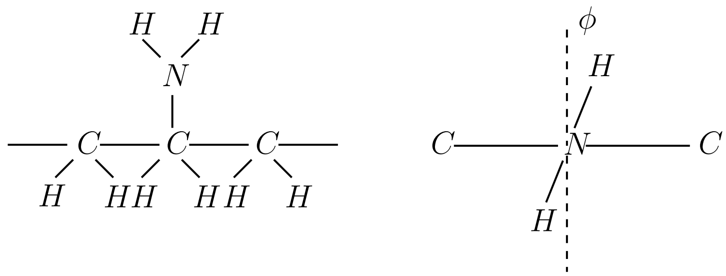
the identity matrix and a standard Cartesian choice. A general wavefunction is then represented as a *complex* fourier series:

$$\psi(\phi) = \sum_{-\infty}^{\infty} a_n \psi_n(\phi)$$

where the $a_n$ are complex coefficients.

**Example: A symmetric $NH_2$ group.**

We can readily envisage a carbon chain with an $NH_2$ group 'dangling' off at some point.



If the molecule is assumed symmetric, then we can consider the rotations of the $NH_2$ group about the $C - N$ bond in isolation with a single azimuthal angle, $\phi$. The kinetic energy will be:

$$K[\phi] = \frac{\left[\hat{L}_\phi\right]^2}{2I}$$

where $\hat{L}_\phi$ is the azimuthal angular momentum and $I$ is the moment of inertia of the $NH_2$ group. As the 'molecule' rotates, it will feel a repulsion from the electrons in the carbon backbone, which to leading order might be modeled by:

$$V[\phi] = -V\cos(2\phi)$$

where the inversion symmetry eliminates the $\cos(\phi)$ term. Rescaling using, $\alpha^2 = 2IV/\hbar^2$ leads to an effective Hamiltonian:

$$H = -\frac{d^2}{d\phi^2} - \alpha^2\cos(2\phi)$$

which can be investigated with a fourier series in the limit $\alpha \mapsto 0$.

# Chapter 16

# Asymptotics: The 'WKB' Approximation

The first step in solving these differential equations is to extract the asymptotic behaviour. All normalisable solutions have special behaviour at the 'edge' of the system and we have to find it.

There are several ways to proceed:

(i) Guess the answer (or at least the form for it)

(ii) Eliminate 'small looking' terms and solve or guess.

(iii) The 'WKB' approximation.

## 16.1 Example: Simple harmonic oscillator

Let us use the one-diemnsional simple harmonic oscillator as an example:

$$-\frac{1}{2}\frac{d^2\psi}{dx^2} + \frac{x^2}{2}\psi = \epsilon\psi$$

(i) Each differenial brings down an $x$, so $\psi \sim e^{\pm(1/2)x^2}$

(ii) $2\epsilon\psi(x) << x^2\psi(x)$ as $x \to \pm\infty$ so look at

$$\frac{d^2\psi}{dx^2} = x^2\psi$$

instead.

$$\left[\frac{d}{dx}+x\right]\left[\frac{d}{dx}-x\right]=\frac{d^2\psi}{dx^2}-x^2-1$$

so look to

$$\frac{d\psi}{dx}=x\psi$$

$$\left[\frac{d}{dx}-x\right]\left[\frac{d}{dx}+x\right]=\frac{d^2\psi}{dx^2}-x^2-1$$

so look to

$$\frac{d\psi}{dx}=-x\psi$$

and $\psi \sim e^{\pm(1/2)x^2}$ again.

(iii) WKB

In the WKB approximation you try the substitution:

$$\psi(x)=e^{-\phi(x)}$$

and then

$$\frac{d^2\psi}{dx^2}=e^{-\phi}\left[\left(\frac{d\phi}{dx}\right)^2-\frac{d^2\phi}{dx^2}\right]\mapsto e^{-\phi}\left(\frac{d\phi}{dx}\right)^2$$

where the final omission constitutes the approximation. A second order differential equation is replaced by a first order equation which is solvable in terms of an elementary integral.

The approximation is good, provided that

$$|\left[\frac{d^2\phi}{dx^2}\left(\frac{d\phi}{dx}\right)^{-2}\right]|\ll 1.$$

For the present case, $\left(\frac{d\phi}{dx}\right)^2=x^2-2\epsilon\sim x^2$ asymptotically. So $\frac{d\phi}{dx}\sim\pm x$ and $\phi\sim\pm\frac{1}{2}x^2$. The previous result is recovered, $\psi(x)\sim e^{\pm x^2/2}$. Note that $\frac{d\phi}{dx}\sim\pm x$ and $\frac{d^2\phi}{dx^2}\sim\pm 1$ so:

$$|\left[\frac{d^2\phi}{dx^2}\left(\frac{d\phi}{dx}\right)^{-2}\right]| \sim \frac{1}{x^2} \ll 1$$

asymptotically.

Once the asymptotic behaviour is found, it is then extracted by substitution. Yet set

$$\psi(x) = A(x)P(x)$$

where $A(x)$ is the convergent asymptotic behaviour found.

For the present case

$$\psi(x) = e^{-x^2/2}P(x)$$

$$\frac{d\psi}{dx} = e^{-x^2/2}\left(\frac{dP}{dx} - xP\right)$$

$$\frac{d^2\psi}{dx^2} = e^{-x^2/2}\left(\frac{d^2P}{dx^2} - 2x\frac{dP}{dx} + (x^2-1)P\right) = (x^2 - 2\epsilon)P$$

and so

$$\frac{d^2P}{dx^2} - 2x\frac{dP}{dx} + (2\epsilon - 1)P = 0 \tag{16.1}$$

is the equation satisfied by the 'residual' part of $\psi(x)$.

Note that this is identical to the equation that the Hermite polynomials satisfy, with $2\epsilon - 1 = 2n$ for integer $n$. We have already solved this problem.

What happen if we look for further asymptotic behaviour? Apply WKB again: $P(x) = e^{-\phi(x)}$

$$\frac{dP}{dx} = -\frac{d\phi}{dx}e^{-\phi}$$

$$\frac{d^2P}{dx^2} = \left[\left(\frac{d\phi}{dx}\right)^2 - \frac{d^2\phi}{dx^2}\right]e^{-\phi} \mapsto \left(\frac{d\phi}{dx}\right)^2 e^{-\phi}$$

so equation (16.1) becomes

$$\left(\frac{d\phi}{dx}\right)^2 + 2x\frac{d\phi}{dx} + 2\epsilon - 1 = 0$$

rearranged

$$\left(\frac{d\phi}{dx} + x\right)^2 = x^2 - 2\epsilon + 1$$

leads to

$$\frac{d\phi}{dx} + x = \pm x\left[1 + \frac{1-2\epsilon}{x^2}\right]^{\frac{1}{2}} \rightarrow \pm\left[x + \frac{1-2\epsilon}{2x} + \dots\right]$$

Yielding two possibilities

(a) $\frac{d\phi}{dx} = -2x$ and so $\phi = -x^2$ and $P(x) \sim e^{x^2}$ which takes us to $\psi \sim e^{x^2/2}$ as before.

(b) $\frac{d\phi}{dx} = \frac{1-2\epsilon}{2x}$ and hence $\phi = -\left(\epsilon - \frac{1}{2}\right)\ln x$ and finally $P(x) \sim e^{-\phi} \sim x^{(\epsilon-1/2)}$ - a power law. Once you reach the situation where you find a power-law, stop and search for a polynomial or series solution.

## 16.2 WKB: Bound-state Aside

What does the WKB approximation tell us about elementary quantum mechanical problems? Let us take as an example a one dimensional potential:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = \epsilon\psi. \tag{16.2}$$

If we assume a WKB solution:

$$\begin{aligned} \psi &= e^{-\phi} \\ \frac{d\psi}{dx} &= -\frac{d\phi}{dx}\psi \\ \frac{d^2\psi}{dx^2} &= \left[\left(\frac{d\phi}{dx}\right)^2 - \frac{d^2\phi}{dx^2}\right]\psi \end{aligned} \tag{16.3}$$

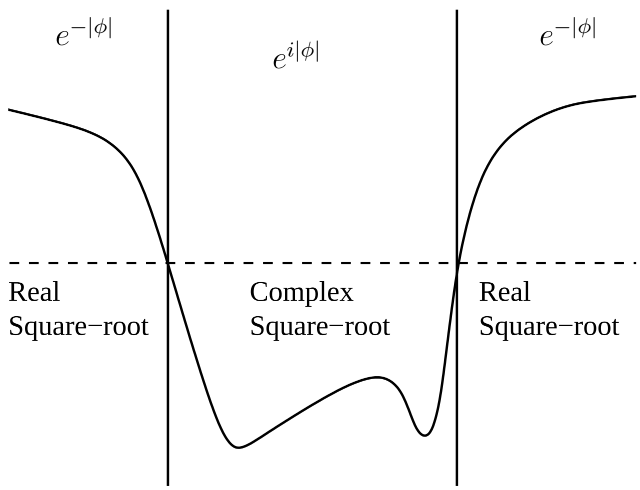
then ignoring the second derivative of $\phi(x)$, we find (16.2) reduces to

$$\left[\frac{d\phi}{dx}\right]^2 = \frac{2m}{\hbar^2}(V(x) - \epsilon) \tag{16.4}$$

and integrating:

$$\phi(x) = \int^x dx' \left[\frac{2m}{\hbar^2}(V(x') - \epsilon)\right]^{\frac{1}{2}}. \tag{16.5}$$

Picture the potential:



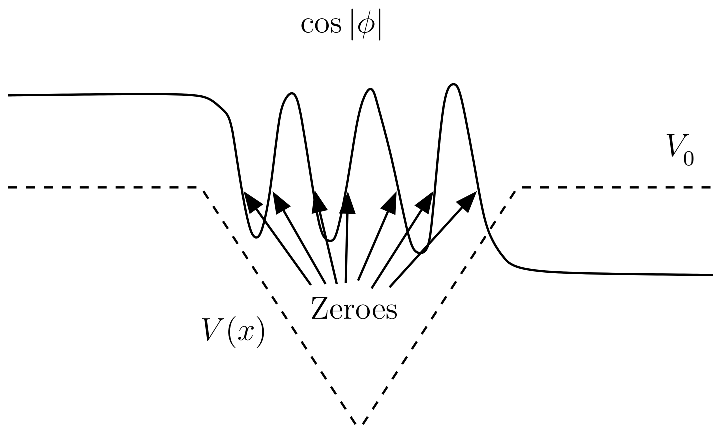

In the region where the potential is above the energy $\epsilon$, the square root is real and we find a real $\phi$ and a wavefunction with no nodes - in this region (16.5) monotonically increasing/decreasing, and if $\phi(x)$ is monotonically increasing the $e^{-\phi(x)}$ .

In the region where the potential is below the energy $\epsilon$, the square root is complex and the solution is oscillating:

$$\psi \sim e^{i|\phi|} = \cos|\phi| + i\sin|\phi|. \tag{16.6}$$

These oscillations provide nodes in the wavefunction and allow us to count the approximate number of bound states below this energy. For the case of a flat potential outside of someregion, and placing the energy at this flat potential, we find a constant wavefunction outside that region:

and we can readily count the number of nodes using:




$$\tilde{\phi} = \int_{x_1}^{x_2} dx \left[ \frac{2m}{\hbar^2}(V_0 - V(x)) \right]^{\frac{1}{2}} \sim n\pi \tag{16.7}$$

there are about $n$ nodes and hence about $n$ bound states!

### 16.2.1 Example: Triangular Potential

If we have a 'triangular' potential:

$$V(x) = -V_1 \Theta(x+a)\Theta(-x)(x+a) - V_2 \Theta(x)\Theta(a-x)(a-x) \tag{16.8}$$

then:

$$n\pi \sim \overline{\phi} = 2\int_0^a dx \left[ \frac{2m}{\hbar^2} V_1 (a-x) \right]^{\frac{1}{2}} = 2 \left[ \frac{2mV_1}{\hbar^2} \right]$$

For an arbitrary triangular potential:

$$V(x) = V_1 |x|$$

we can include an energy, $E$, and attempt to assess the number of states below that energy using the previous argument. We use the assignment:

$$V_1 x - E \equiv -V_1(a-x)$$

to deduce that the number of states scales as:

$$n\pi \sim 2\left[\frac{2mV_1}{\hbar^2}\right]^{\frac{1}{2}}\frac{2}{3}\left[\frac{E}{V_1}\right]^{3/2}$$

and so:

$$E \sim \left[\frac{3\hbar V_1 \pi}{4[2m]^{1/2}}\right]^{\frac{2}{3}} n^{2/3}$$

and the energy increases with a strange power of the number of states!

## 16.3 The Hydrogen Atom: Asymptotics

We apply the same ideas to the hydrogen atom,

$$\frac{d^2\psi}{dr^2} + \frac{2}{r}\frac{d\psi}{dr} - \frac{l(l+1)}{r^2}\psi + \frac{2}{r}\psi + \epsilon\psi = 0. \tag{16.9}$$

we wish to substitution $\psi(r) = r^l\Psi(r)$, the terms would become

$$\begin{aligned}\frac{d^2\psi}{dr^2} &= \frac{d^2}{dr^2}(r^l\Psi) = r^l\frac{d^2\Psi}{dr^2} + 2lr^{l-1}\frac{d\Psi}{dr} + l(l-1)r^{l-2}\Psi \\ \frac{d\psi}{dr} &= \frac{d}{dr}(r^l\Psi) = r^l\frac{d\Psi}{dr} + lr^{l-1}\Psi\end{aligned}$$

using these we obtain:

$$\begin{aligned}& \frac{d^2\psi}{dr^2} + \frac{2}{r}\frac{d\psi}{dr} - \frac{l(l+1)}{r^2}\psi \\ = & \left[\left(r^l\frac{d^2\Psi}{dr^2} + 2lr^{l-1}\frac{d\Psi}{dr} + l(l-1)r^{l-2}\Psi\right) + \frac{2}{r}\left(r^l\frac{d\Psi}{dr} + lr^{l-1}\Psi\right) - l(l+1)r^{l-2}\Psi\right] \\ = & \; r^l\left[\frac{d^2\Psi}{dr^2} + \frac{2(l+1)}{r}\frac{d\Psi}{dr}\right] \qquad (16.10)\end{aligned}$$

which simplifies things and does not affect the potential.

$$\frac{d^2\Psi}{dr^2} + \frac{2(l+1)}{r}\frac{d\Psi}{dr} + \frac{2}{r}\Psi + \epsilon\Psi = 0. \tag{16.11}$$

Now using WKB ($\Psi = e^{-\phi}$)

$$\left(\frac{d\phi}{dr}\right)^2 - 2\frac{l+1}{r}\frac{d\phi}{dr} + \frac{2}{r} + \epsilon = 0$$

rearranged

$$\left(\frac{d\phi}{dr} - \frac{l+1}{r}\right)^2 = -\epsilon - \frac{2}{r} + \frac{(l+1)^2}{r^2}$$

and $r \to \infty$ limit, $\frac{d\phi}{dr} \to \pm\sqrt{\epsilon}$ and $\phi \pm \sqrt{\epsilon}r$. We only get bound states with $\epsilon < 0$ and using $\epsilon = -\alpha^2$ we find $\Psi(r) = e^{-\alpha r}P(r)$ extracts the asymptotics. Substituting this into the terms of (16.11)

$$\frac{d^2\Psi}{dr^2} = \frac{d^2}{dr^2}[e^{-\alpha r}P(r)] = e^{-\alpha r}\frac{d^2P}{dr^2} - 2\alpha e^{-\alpha r}\frac{dP}{dr} + \alpha^2 e^{-\alpha r}P$$
$$\frac{d\Psi}{dr} = \frac{d}{dr}(e^{-\alpha r}P) = e^{-\alpha r}\frac{dP}{dr} - \alpha e^{-\alpha r}P$$

Then (16.11) becomes

$$\left(\frac{d^2P}{dr^2} - 2\alpha\frac{dP}{dr} + \alpha^2 P\right) + \frac{2(l+1)}{r}\left(\frac{dP}{dr} - \alpha P\right) + \frac{2}{r}P - \alpha^2 P = 0$$

or

$$r\frac{d^2P}{dr^2} + 2\left(l+1-\alpha r\right)\frac{dP}{dr} + 2\left(1-(l+1)\alpha\right)P = 0$$

which is an equation quite similar to Laguerre's.

It is usual to rescale the radius $r$, by $r = \frac{\rho}{2\alpha}$ and then:

$$\rho\frac{d^2P}{dr^2} + (2(l+1)-\rho)\frac{dP}{dr} + \left[\frac{1}{\alpha} - 1 - l\right]P = 0 \tag{16.12}$$

and this is even closer to Laguerre's equation, i.e:

$$x\frac{d^2L}{dx^2} + (1-x)\frac{dL}{dx} + sL = 0$$

and if we consider

$$L_n(x) \equiv \frac{d^n L}{dx^n}$$

then using Leibnitz

$$\begin{aligned}
& \left(\frac{d}{dx}\right)^n \left[x\frac{d^2L}{dx^2} + (1-x)\frac{dL}{dx} + sL\right] \\
= \quad & x\frac{d^2L_n}{dx^2} + n\frac{dL_n}{dx} + (1-x)\frac{dL}{dx} - nL_n + sL_n = 0 \qquad (16.13)
\end{aligned}$$

or

$$x\frac{d^2L_n}{dx^2} + (n+1-x)\frac{dL_n}{dx} + (s-n)L_n = 0 \qquad (16.14)$$

Comparing (16.12) with (16.14), $L_n$ solves the problem provided that $2(l+1) = n+1$ and $s - n = \frac{1}{\alpha} - l - 1 \geq 0$

## 16.4 Spherical Harmonics: Asymptotics

The generating equation is:

$$\left(-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}\right] + \frac{m^2}{\sin^2\theta}\right)\psi_\theta = l(l+1)\psi_\theta \qquad (16.15)$$

but usually the transformation $u = \cos\theta$ is employed to provide:

$$\left(\frac{d}{du}\left[(1-u^2)\frac{d}{du}\right] - \frac{m^2}{1-u^2} + l(l+1)\right)\psi(u) = 0 \qquad (16.16)$$

Obviously, the 'edge' of the system is $u = \pm 1$ and there (16.16) is

$$\frac{d}{du}\left[(1-u^2)\frac{d}{du}\right]\psi(u) \sim \frac{m^2}{1-u^2}\psi(u) \qquad (16.17)$$

and the natural asymptotic behaviour is

$$\psi(u) \sim (1-u^2)^\alpha \qquad (16.18)$$

for some $\alpha$. With this assumption

$$\frac{d\psi}{du} \sim -2\alpha(1-u^2)^{\alpha-1}u$$

$$\begin{aligned}
\frac{d}{du}\left[(1-u^2)\frac{d}{du}\right]\psi &= \frac{d}{du}\left[-2\alpha(1-u^2)^{\alpha}u\right] \\
&= 4\alpha^2u^2(1-u^2)^{\alpha-1} - 2\alpha(1-u^2)^{\alpha} \\
&= 4\alpha^2(1-u^2)^{\alpha-1} - 2\alpha(2\alpha+1)(1-u^2)^{\alpha} \qquad (16.19)
\end{aligned}$$

so to leading order we need $4\alpha^2 = m^2$ in order to satisfy (16.17). Extracting the asymptotics , i.e. $\psi(u) = (1-u^2)^{m/2}P(u)$, yields:

$$\frac{d\psi}{du} = (1-u^2)^{m/2}\frac{dP}{du} - mu(1-u^2)^{(m-2)/2}P(u)$$

$$\begin{aligned}
\frac{d}{du}\left[(1-u^2)\frac{d}{du}\right]\psi &= \frac{d}{du}\left[(1-u^2)^{(m+2)/2}\frac{dP}{du} - mu(1-u^2)^{m/2}P(u)\right] \\
&= (1-u^2)^{(m+2)/2}\frac{d^2P}{du^2} - u(m+1)(1-u^2)^{m/2}\frac{dP}{du} \\
&- mu(1-u^2)^{m/2}\frac{dP}{du} + m^2u^2(1-u^2)^{(m-2)/2}P \\
&- m(1-u^2)^{m/2}P \qquad (16.20)
\end{aligned}$$

and sustituting this into (16.16) gives

$$\begin{aligned}
&\left[(1-u^2)^{(m+2)/2}\frac{d^2P}{du^2} - 2(m+1)u(1-u^2)^{m/2}\frac{dP}{du}\right. \\
&\qquad \left. + m(1-u^2)^{m/2}\left(\frac{mu^2}{(1-u^2)} - 1\right)P\right] \\
&-\left(\frac{m^2}{1-u^2} + l(l+1)\right)(1-u^2)^{m/2}P(u) = 0
\end{aligned}$$

or

$$(1-u^2)\frac{d^2P}{du^2} - 2(m+1)u\frac{dP}{du} + [l(l+1) - m(m+1)]P = 0 \qquad (16.21)$$

We are left with three differential equations with asymptotics extracted, which we can finally solve using the *series solution* method.

# Chapter 17

# Series Solutions

When you have extracted the symptotics and are expecting a polynomial solution,the 'simplest' method of solving the problem is via a series solution.

The idea is simple: Assume that:

$$P(x) = \sum_{m=0}^{\infty} a_m x^{m+\sigma} \tag{17.1}$$

with $a_0 \neq 0$,and then substitute this into the equation and determine both $\sigma$, the initial power of $x$, and a recurrence relationship between the coefficients $a_m$. The eigenvalues and corresponding eigenstates occur when the polynomial terminates, i.e. is finite.

The best way to understand is by example:

## 17.1 Simple-Harmonic Oscillator: Series solution

The governing equation is:

$$\frac{d^2P}{dx^2} - 2x\frac{dP}{dx} + (2\epsilon - 1)P = 0. \tag{17.2}$$

The crucial step is to see how each term scales:

$$\frac{d^2P}{dx^2} \sim \frac{P}{x^2}$$

$$x\frac{dP}{dx} \sim P.$$

and then provided that there are onlytwo typesof scaling, separate them to opposite sides of the equation

$$\frac{d^2P}{dx^2} - 2x\frac{dP}{dx} + (2\epsilon - 1)P.$$

Substitute in the assumption

$$\begin{aligned}\frac{d^2P}{dx^2} &= \sum_{m=0}^{\infty} a_m(m+\sigma)(m+\sigma-1)x^{m+\sigma-2} \\ &= \sigma(\sigma-1)a_0x^{\sigma-2} + (\sigma+1)\sigma a_1x^{\sigma-1} + (\sigma+2)(\sigma+1)a_2x^{\sigma} + \dots \end{aligned} \tag{17.3}$$

$$\begin{aligned}2x\frac{dP}{dx} + (1-2\epsilon) &= \sum_{m=0}^{\infty} a_m[2(m+\sigma)+1-2\epsilon]x^{m+\sigma} \\ &= [2\sigma+1-2\epsilon]a_0x^{\sigma} + [2\sigma+3-2\epsilon]a_1x^{\sigma+1} + \dots \end{aligned} \tag{17.4}$$

Since the different types of term scale differently, one sequence will start before the other. These unbalanced contributions must vanish, and this usually defines $\sigma$.

Currently, $\frac{d^2P}{dx^2}$ has terms in $x^{\sigma-2}$ and $x^{\sigma-1}$ which have no counterparts, so

$$\sigma(\sigma-1)a_0 = 0, \qquad (\sigma+1)\sigma a_1 = 0. \tag{17.5}$$

This tells us that $\sigma = 0$ or $\sigma = 1$ if $a_0 \neq 0$ In fact, it is quite clever to use $\sigma = 0$ to solve both, and then either $a_0 \neq 0$ and $a_1 = 0$ or $a_0 = 0$ and $a_1 \neq 0$ as we will shall see later on. Once we have found $\sigma$, we may substitute it into (17.3) and (17.4):

$$\frac{d^2P}{dx^2} = \sum_{m=0}^{\infty} a_m m(m-1)x^{m-2} = 2a_2 + 6a_3x + \dots \tag{17.6}$$

$$2x\frac{dP}{dx} + (1-2\epsilon) = \sum_{m=0}^{\infty} a_m[2m+1-2\epsilon]x^m = [1-2\epsilon]a_0 + [3-2\epsilon]a_1x + [5-2\epsilon]a_2x^2 + \dots \tag{17.7}$$

We see that

$$\begin{aligned} 2a_2 &= a_0[1 - 2\epsilon] \\ 6a_3 &= a_1[3 - 2\epsilon] \end{aligned}$$

and so on...

We immediately see from (17.7) that the sequence can terminate when there is $2N+1 = 2\epsilon$ for some integer $n$ so

$$\epsilon = N + \frac{1}{2}$$

are the eigenvalues.

To evaluate the coefficients, however, we need to find the recurrence relationship. This is best done by relabelling the summation:

$$\frac{d^2P}{dx^2} = \sum_{m=0}^{\infty} a_m m(m-1)x^{m-2} = \sum_{n=-2}^{\infty} a_n (n+2)(n+1)x^n$$

$$\frac{d^2P}{dx^2} = \sum_{n=0}^{\infty} a_n [2n + 1 - 2\epsilon]x^n$$

and so:

$$(n+2)(n+1)a_{n+2} = [2n + 1 - 2\epsilon]a_n \tag{17.8}$$

is the recurrence relationship providing us with the $a_n$. The sequence terminates if $\epsilon = N + \frac{1}{2}$ for some integer $N$, and then:

$$a_{n+2}^{(N)} = (-1)\frac{2(N-n)}{(n+2)(n+1)}a_n^{(N)} \tag{17.9}$$

Note that these terms are either all even, if $N$ is even, or all odd, if $N$ is odd.

## 17.2 Hydrogen Atom: Series Solution

We will now look at the Hydrogen atom,armed with the technique. The governing equations is:

$$\rho\frac{d^2P}{d\rho^2} + (2(l+1) - \rho)\frac{dP}{d\rho} + \left[\frac{1}{\alpha} - 1 - l\right] P = 0. \tag{17.10}$$

First analyse the scaling of the terms:

$$\rho\frac{d^2P}{d\rho^2} \sim \frac{P}{\rho}$$

$$\frac{dP}{d\rho} \sim \frac{P}{\rho}$$

$$\rho\frac{dP}{d\rho} \sim P$$

so there are two types of term and:

$$\rho\frac{d^2P}{d\rho^2} + 2(l+1)\frac{dP}{d\rho} = \rho\frac{dP}{d\rho} + \left[1 + l - \frac{1}{\alpha}\right] P$$

Assume:

$$P = \sum_{m=0}^{\infty} a_m \rho^{m+\sigma} \tag{17.11}$$

and then

$$\begin{aligned} \rho\frac{d^2P}{d\rho^2} + 2(l+1)\frac{dP}{d\rho} &= \sum_{m=0}^{\infty} a_m[(m+\sigma)(m+\sigma-1) + 2(1+l)(m+\sigma)]\rho^{m+\sigma-1} \\ &= \sum_{m=0}^{\infty} a_m(m+\sigma)(m+\sigma+1+2l)\rho^{m+\sigma-1} \end{aligned} \tag{17.12}$$

$$\rho\frac{dP}{d\rho} + \left[1 + l - \frac{1}{\alpha}\right] P = \sum_{m=0}^{\infty} a_m \left[m + \sigma + 1 + l - \frac{1}{\alpha}\right] \rho^{m+\sigma} \tag{17.13}$$

The top series has one additional term (corresponding to $m = 0$). Forcing this term to vanish yields:

$$a_0 \sigma[\sigma + 1 + 2l] = 0 \tag{17.14}$$

so $\sigma = 0$ or $\sigma = -1 - 2l$. The second case is horribly diveregent. ...

Put $\sigma = 0$

$$\rho \frac{d^2 P}{d\rho^2} + 2(l+1)\frac{dP}{d\rho} = \sum_{m=0}^{\infty} a_m m(m+1+2l)\rho^{m-1} = \sum_{n=-1}^{\infty} a_{n+1}(n+1)(n+2+2l)\rho^n \tag{17.15}$$

$$\rho \frac{dP}{d\rho} + \left[1 + l - \frac{1}{\alpha}\right] P = \sum_{n=0}^{\infty} a_n \left[n + 1 + l - \frac{1}{\alpha}\right] \rho^n \tag{17.16}$$

The eigenvalues occur when

$$\frac{1}{\alpha} = N + 1 + l$$

for some integer $N$. Comparing (17.15) and (17.16) we obtain

$$a_{n+1}(n+1)(n+2+2l) = a_n \left[n + 1 + l - \frac{1}{\alpha}\right] \rho^n$$

and the sequence terminates if $\frac{1}{\alpha} = N + l + 1$ and then

$$a_{n+1}^{(N)} = (-1)\frac{(N-n)}{(n+1)(n+2+2l)} a_n^{(N)} \tag{17.17}$$

to find the eigenfucntions.

## 17.3 Spherical-Harmonics: Series Solution

The governing equation is:

$$(1-u^2)\frac{d^2 P}{du^2} + 2(m+1)u\frac{dP}{du} + [l(l+1) - m(m+1)]P = 0. \tag{17.18}$$

First, look at the scaling:

$$\frac{d^2P}{du^2} \sim \frac{P}{u^2}$$

$$u^2\frac{d^2P}{du^2} \sim P$$

$$u\frac{dP}{du} \sim P$$

so again there are two types of term and:

$$\frac{d^2P}{du^2} = u^2\frac{d^2P}{du^2} + 2(m+1)u\frac{dP}{du} - [l(l+1) - m(m+1)]P$$

Assume:

$$P = \sum_{n=0}^{\infty} a_n u^{n+\sigma}$$

and then

$$\frac{d^2P}{du^2} = \sum_{n=0}^{\infty} a_n(n+\sigma)(n+\sigma-1)u^{n+\sigma-2} \tag{17.19}$$

$$\begin{aligned} & u^2\frac{d^2P}{du^2} + 2(m+1)u\frac{dP}{du} - [l(l+1) - m(m+1)]P \\ = & \sum_{n=0}^{\infty} a_n[(n+\sigma)(n+\sigma-1) + 2(m+1)(n+\sigma) - (l-m)(l-m+1)]u^{n+\sigma} \end{aligned} \tag{17.20}$$

Similar to the Harmonic Oscillator there are two terms uncompesated, so:

$$\sigma(\sigma-1) = 0, \qquad (\sigma-1)\sigma a_1 = 0 \tag{17.21}$$

which is identical to before, and so we choose $\sigma = 0$ and allow $a_0 = 0$ if desired.

$$\frac{d^2P}{du^2} = \sum_{n=0}^{\infty} a_n n(n-1)u^{n-2} = \sum_{n=-2}^{\infty} a_{n+2}(n+2)(n+1)u^n \tag{17.22}$$

$$\begin{aligned}
& u^2\frac{d^2P}{du^2} + 2(m+1)u\frac{dP}{du} - [l(l+1) - m(m+1)]P \\
= & \sum_{n=0}^{\infty} a_n[n(n-1) + 2(m+1)n - (l-m)(l-m+1)]u^n \\
= & \sum_{n=0}^{\infty} a_n(n-l+m)(n+l+m+1)u^n
\end{aligned} \tag{17.23}$$

and so the 'eigenvalues' involve $l - m$ being a positive integer:

$$a_{n+2}^{(lm)} = (-1)\frac{(l-m-n)(l+m+n+1)}{(n+2)(n+1)}a_n^{(lm)} \tag{17.24}$$

which can be used for the eigenfucntions.

# Chapter 18

# Generating Functions

## 18.1 Simple-Harmonic Oscillator

The generating function

$$G(x,t) = e^{-t^2+2xt} = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(x) \tag{18.1}$$

where $H_n(x)$ are the Hermite polynomials.

We note that it is easy to obtain this formula from

$$H_n(x) = (-1)^n e^{x^2} \left[\frac{d}{dx}\right]^n e^{-x^2} \tag{18.2}$$

(where here we have incuded a term $(-1)^n$ so as to make the higest order term to have a positive coefficient) by introducing a dummy variable $t$ and writing

$$H_n(x) = e^{x^2} \left[\frac{\partial}{\partial t}\right]^n e^{-(x-t)^2}\Big|_{t=0} = \left[\frac{\partial}{\partial t}\right]^n e^{2x-t^2}\Big|_{t=0} \tag{18.3}$$

as this implies a Taylor expansion around $t = 0$, which is precisely (18.1).

### 18.1.1 Explicit Form of Hermite Polynomials via Generating Function

From the generating function we can derive an explicit expression for the Hermite polynomials:

$$H_n(x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k \frac{n!}{k!(n-2k)!}(2x)^{n-2k} \tag{18.4}$$

We start by expanding out the generating function,

$$e^{-t^2+2xt} = 1 + t(2x-t) + \frac{1}{2!}t^2(2x-t)^2 + \frac{1}{3!}t^3(2x-t)^3 + \ldots . \tag{18.5}$$

To obtain $H_n(x)$ we need to find the coefficient of $\frac{t^n}{n!}$. Contributions come from the term $\frac{1}{n!}t^n(2x-t)^n$ and those terms below it. We will need the binomial expansion

$$(2x-t)^m = \sum_{q=0}^{m} \frac{m!}{q!(m-q)!}(-t)^q(2x)^{m-q}. \tag{18.6}$$

From the term $\frac{1}{n!}t^n(2x-t)^n$ we get the contribution to $\frac{t^n}{n!}$ ($m = n$ and $q = 0$ term in (18.6)):

$$(2x)^n.$$

From the next lower term $\frac{1}{(n-1)!}t^{n-1}(2x-t)^{n-1}$ we get the contribution to $\frac{t^n}{n!}$ ($m = n-1$ and $q = 1$):

$$n!\left[\frac{1}{(n-1)!} \times \frac{(n-1)!}{1!(n-2)!}(-1)(2x)^{n-2}\right] = (-1)\frac{n!}{1!(n-2)!}(2x)^{n-2}.$$

From the next lower term $\frac{1}{(n-2)!}t^{n-2}(2x-t)^{n-2}$ we get the contribution to $\frac{t^n}{n!}$ ($m = n-2$ and $q = 2$):

$$n!\left[\frac{1}{(n-2)!} \times \frac{(n-2)!}{2!(n-4)!}(-1)^2(2x)^{n-4}\right] = (-1)^2\frac{n!}{2!(n-4)!}(2x)^{n-4}.$$

From the general term $\frac{1}{(n-k)!}t^{n-k}(2x-t)^{n-k}$ we get the contribution to $\frac{t^n}{n!}$ ($m = n-k$ and $q = k$):

$$n!\left[\frac{1}{(n-k)!}\times\frac{(n-k)!}{k!(n-2k)!}(-1)^k(2x)^{n-2k}\right]=(-1)^k\frac{n!}{2!(n-2k)!}(2x)^{n-2k}.$$

The series terminates at $k=\lfloor\frac{n}{2}\rfloor$ and we have established (18.4). We also prove this result by induction after deriving somerecurrence relations in the next section.

### 18.1.2 Recurrence relations

We can use the generating function to derive so recurrence relations:

(i)

$$H_{n+1}(x)=2xH_n(x)-2nH_{n-1}(x) \tag{18.7}$$

where we define $H_{-1}=0$.

(ii)

$$\frac{d}{dx}H_n(x)=2nH_{n-1}(x) \tag{18.8}$$

(iii)

$$H_{n+1}(x)-2xH_n(x)+\frac{d}{dx}H_{n-1}(x)=0. \tag{18.9}$$

**Proof**:

(i) First consider

$$\frac{\partial}{\partial t}G(x,t)=2(x-t)e^{-t^2+2xt}=\sum_{n=0}^{\infty}\frac{t^{n-1}}{(n-1)!}H_n(x) \tag{18.10}$$

Using

$$\sum_{n=0}^{\infty}\frac{t^{n-1}}{(n-1)!}H_n(x)=\sum_{n=0}^{\infty}\frac{t^n}{n!}H_{n+1}(x)$$

and

$$
\begin{aligned}
-2te^{-t^2+2xt} &= -2\sum_{n=0}^{\infty}\frac{t^{n+1}}{n!}H_n(x) \\
&= -2\sum_{n=1}^{\infty}\frac{t^n}{n!}nH_{n-1}(x)
\end{aligned}
$$

in (18.10)

$$
2\sum_{k=0}^{\infty}\frac{t^n}{n!}xH_n(x) - 2\sum_{k=1}^{\infty}\frac{t^n}{n!}nH_{n-1}(x) = \sum_{k=0}^{\infty}\frac{t^n}{n!}xH_{n+1}(x)
$$

and equating coeficients we obtain (18.7).

(ii) Differentiating with respect to $x$:

$$
\frac{\partial}{\partial x}G(x,t) = 2te^{-t^2+2xt} = \sum_{n=0}^{\infty}\frac{t^n}{n!}\frac{d}{dx}H_n(x)
$$

from which we immediatly get

$$
2\sum_{n=0}^{\infty}\frac{t^n}{n!}nH_{n-1}(x) = \sum_{n=0}^{\infty}\frac{t^n}{n!}\frac{d}{dx}H_n(x)
$$

and upon equating coefficients obtain (18.8).

(iii) The relation (18.9) is obtained by substituting (18.8) into (18.7)

### 18.1.3 Explicit Form of Hermite Polynomials: Proof by induction

$$
H_n(x) = \sum_{k=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^k\frac{n!}{k!(n-2k)!}(2x)^{n-2k} \tag{18.11}
$$

We use the reccursive relation (18.7):

$$
H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)
$$

$$H_{n+1}(x) = 2x\sum_{k=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^k\frac{n!}{k!(n-2k)!}(2x)^{n-2k} - 2n\sum_{k=0}^{\lfloor\frac{n-1}{2}\rfloor}(-1)^k\frac{(n-1)!}{k!(n-1-2k)!}(2x)^{n-1-2k} \tag{18.12}$$

and write $k' = k - 1$ in the second summation

$$\sum_{k=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^k\frac{n!}{k!(n-2k)!}(2x)^{n+1-2k} - 2\sum_{k'=1}^{\lfloor\frac{n-1}{2}\rfloor+1}(-1)^{k'-1}\frac{n!}{(k'-1)!(n+1-2k')!}(2x)^{n+1-2k'} \tag{18.13}$$

For $n$ even $\lfloor\frac{n-1}{2}\rfloor + 1 = \lfloor\frac{n}{2}\rfloor$ and for $n$ odd $\lfloor\frac{n-1}{2}\rfloor + 1 = \frac{n+1}{2} = \lfloor\frac{n+1}{2}\rfloor$.

We deal with even case first:

Separating out the $k = 0$ term in the first summation and replacing $k'$ by $k$ we obtain

$$(-1)^0\frac{n!}{0!(n-0)!}(2x)^{n+1-0} + \sum_{k=1}^{\lfloor\frac{n}{2}\rfloor}(-1)^k\left[\frac{n!}{k!(n-2k)!} + 2\frac{n!}{(k-1)!(n+1-2k)!}\right](2x)^{n+1-2k} \tag{18.14}$$

The term in the square brackets simplify:

$$\frac{n!}{k!(n+1-2k)!}\big\{(n+1-2k) + 2k\big\} = \frac{(n+1)!}{k!(n+1-2k)!}$$

and for the isolated term:

$$(-1)^0\frac{n!}{0!n!}(2x)^{n+1} = (2x)^{n+1} = (-1)^0\frac{(n+1)!}{0!(n+1-2\times 0)!}(2x)^{n+1-2\times 0}$$

and so we have for (18.14)

$$H_{n+1}(x) = \sum_{k=0}^{\lfloor\frac{n}{2}\rfloor}(-1)^k\frac{(n+1)!}{k!(n+1-2k)!}(2x)^{n+1-2k} \tag{18.15}$$

where we have used $\lfloor\frac{n+1}{2}\rfloor = \frac{n}{2} = \lfloor\frac{n}{2}\rfloor$ for $n$ even.

We now do $n$ odd:

$$
\begin{aligned}
& \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k \frac{(n+1)!}{k!(n+1-2k)!} (2x)^{n+1-2k} + \left( k' = \frac{n+1}{2} \text{ in second part of (18.13)} \right) \\
= \quad & \dots \quad + 2(-1)^{\frac{n+1}{2}} \frac{n!}{(\frac{n+1}{2}-1)!(n+1-2\frac{n+1}{2})!} (2x)^{n+1-2\frac{n+1}{2}} \\
= \quad & \dots \quad + 2(-1)^{\frac{n+1}{2}} \frac{n!}{(\frac{n+1}{2}-1)!(0)!} \qquad (18.16)
\end{aligned}
$$

But we get

$$
\begin{aligned}
(-1)^{\frac{n+1}{2}} \frac{(n+1)!}{(\frac{n+1}{2})!(n+1-2\frac{n+1}{2})!} (2x)^{n+1-2\frac{n+1}{2}} &= 2(-1)^{\frac{n+1}{2}} \frac{n+1}{\frac{n+1}{2}} \frac{n!}{(\frac{n+1}{2}-1)!(0)!} \\
&= 2(-1)^{\frac{n+1}{2}} \frac{n!}{(\frac{n+1}{2}-1)!(0)!}
\end{aligned}
$$

and so we have

$$
H_{n+1}(x) = \sum_{k=0}^{\lfloor \frac{n+1}{2} \rfloor} (-1)^k \frac{(n+1)!}{k!(n+1-2k)!} (2x)^{n+1-2k} \qquad (18.17)
$$

So we have obtained the correct formula, i.e. (18.18) with $n \mapsto n+1$, for both $n$ even and $n$ odd.

Now we can argue that if it works for $n = 1$ and for $n = 2$ then it works for $n = 3$. We then know it works for $n = 2$ and $n = 3$ therefore it works for $n = 4$,and so on...

So for $n = 1$:

$$
\sum_{k=0}^{0} (-1)^0 \frac{1!}{0!(1-2\times 0)!} (2x)^{1-2\times 0} = 2x = H_1(x)
$$

and for $n = 2$:

$$
\sum_{k=0}^{1} (-1)^k \frac{2!}{k!(2-2k)!} (2x)^{2-2k} = 4x^2 - 2 = H_2(x).
$$

$$
H_n(x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k \frac{n!}{k!(n-2k)!} (2x)^{n-2k} \qquad (18.18)
$$

### 18.1.4 Deriving the differential equation for the $H_n(x)$

Differentiating (18.9) we obtain

$$\frac{d^2}{dx^2}H_n(x) - 2x\frac{d}{dx}H_n - 2H_n(x) + \frac{d}{dx}H_{n+1}(x) = 0$$

and using (18.8) to eliminate $H_{n+1}(x)$:

$$\frac{d^2}{dx^2}H_n(x) - 2x\frac{d}{dx}H_n - 2H_n(x) + 2(n+1)H_n(x) = 0$$

which easily simplifies to differential equation for Hermite polynomials:

$$\frac{d^2}{dx^2}H_n(x) - 2x\frac{d}{dx}H_n + 2nH_n(x) = 0.$$

### 18.1.5 Normalisation

Normalisation can be performed analytically using this representation:

$$\begin{aligned}
\int_{-\infty}^{\infty} dx e^{-x^2} e^{-s^2+2xs} e^{-t^2+2xt} &= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{s^n}{n!}\frac{t^m}{m!}\int_{-\infty}^{\infty} e^{-x^2} H_n(x)H_m(x) \\
&= \int_{-\infty}^{\infty} dx e^{-(x-s-t)+2st} \\
&= e^{2st}\int_{-\infty}^{\infty} dx e^{-x^2} \\
&= \sqrt{\pi}e^{2st} \\
&= \sqrt{\pi}\sum_{n=0}^{\infty}\frac{2^n s^n t^n}{n!} \qquad (18.19)
\end{aligned}$$

and so equating terms:

$$\int_{-\infty}^{\infty} dx e^{-x^2} H_n(x)H_m(x) = \delta_{nm}\sqrt{\pi}2^n n!. \qquad (18.20)$$

## 18.2 Electrosstatics: A Single Electron

In electrostatics, there are two governing equations:

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}, \qquad \nabla \times \mathbf{E} = 0. \tag{18.21}$$

The second guarantees the existence of a potential:

$$\mathbf{E} = -\nabla V \tag{18.22}$$

which, when substituted into the first equation provides:

$$\nabla^2 V = -\frac{\rho}{\epsilon_0}. \tag{18.23}$$

If we are dealing with a single electron, then:

$$\rho(\mathbf{x}) = -e\delta(\mathbf{x} - \mathbf{x}_0) \tag{18.24}$$

and we have only at $\mathbf{x}_0$ and nowhere else. Since we know the potential from a single electron, we must have that:

$$\nabla^2_{\mathbf{x}} \left[ \frac{e}{4\pi\epsilon_0 |\mathbf{x} - \mathbf{x}_0|} \right] = -\frac{e}{\epsilon_0}\delta(\mathbf{x} - \mathbf{x}_0) \tag{18.25}$$

a result that will be useful in understanding Legendre poloynomials.

Firstly, let us prove the result. Use spherical polar coordinates cenetered at $\mathbf{x}_0$ as the origin, $\mathbf{x} = \mathbf{x}_0 + \mathbf{r}$:

$$\nabla^2_{\mathbf{x}} = \nabla^2_r = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2}\nabla^2_\Omega$$

where $\nabla^2_\Omega$ is the angular Laplacian:

$$\nabla^2_\Omega = \left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right) = \frac{\partial}{\partial u}(1-u^2)\frac{\partial}{\partial u} + \frac{1}{1-u^2}\frac{\partial^2}{\partial\phi^2}.$$

where $u = \cos\theta$. Applying this to $1/r$ provides

$$\nabla_r^2 \frac{1}{r} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\frac{1}{r} = 0$$

so it is clear that the Laplacian of $1/r$ vanishes everywhere except perhaps at the origin. Toasses any contribution which might be lurking at the origin, we consider a volume integral over a small sphere centred on $\mathbf{x}_0$:

$$L = \int_V dV \nabla^2 \frac{1}{r} = \int_S \mathbf{dS} \cdot \nabla \frac{1}{r}$$

employing the divergence theorem. Using spherical polars and the curvilinear section:

$$\nabla \frac{1}{r} = \hat{\mathbf{r}}\frac{\partial}{\partial r}\left[\frac{1}{r}\right] + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta}\left[\frac{1}{r}\right] + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}\left[\frac{1}{r}\right] = -\frac{\hat{\mathbf{r}}}{r^2}$$

and since $\mathbf{dS} = dA\hat{\mathbf{r}}$ for a sphere:

$$L = (-1)\frac{1}{r^2}\int_S dA = (-1)4\pi$$

and hence there is a contrbution at $\mathbf{x} = \mathbf{x}_0$ and the result (18.25) follows.

## 18.3 Generating Function for Legendre Polynomials

Fot $\mathbf{x} \neq \mathbf{x}_0$, we have

$$\nabla_{\mathbf{x}}^2 \frac{1}{|\mathbf{x} - \mathbf{x}_0|} = 0. \tag{18.26}$$

We employ $\mathbf{x}_0 = \hat{\mathbf{z}}$ and then:

$$\begin{aligned}
|\mathbf{x} - \mathbf{x}_0| &= [(\mathbf{x} - \hat{\mathbf{z}}) \cdot (\mathbf{x} - \hat{\mathbf{z}})]^{\frac{1}{2}} \\
&= [(\hat{\mathbf{z}} \cdot \hat{\mathbf{z}} + \mathbf{x} \cdot \mathbf{x} - 2\mathbf{x} \cdot \hat{\mathbf{z}})]^{\frac{1}{2}} \\
&= [1 + x^2 - 2x\cos\theta]^{\frac{1}{2}} \qquad (18.27)
\end{aligned}$$

and hence:

$$\nabla^2_{\mathbf{x}} \frac{1}{[1+x^2-2x\cos\theta]^{\frac{1}{2}}} = 0 \qquad x \neq 1. \tag{18.28}$$

Expand as a power series in $x$:

$$\nabla^2_{\mathbf{x}} \sum_{l=0}^{\infty} x^l P_l[\cos\theta] = 0 \tag{18.29}$$

and then use polar coordinates in $\mathbf{x}$:

$$\sum_{l=0}^{\infty} \left[ \frac{1}{x^2} \frac{\partial}{\partial x} \left[ x^2 \frac{\partial}{\partial x} \right] + \frac{1}{x^2} \nabla^2_{\Omega} \right] x^l P_l[\cos\theta] = 0 \tag{18.30}$$

and hence

$$\sum_{l=0}^{\infty} \frac{x^l}{x^2} \left[ \nabla^2_{\Omega} + l(l+1) \right] P_l[\cos\theta] = 0 \tag{18.31}$$

and the $P_l[\cos\theta]$ are the Legendre Polynomials.

### 18.3.1 Spherical-Harmonics

The generating function for Legendre polynomials is:

$$[1+t^2-2ut]^{-\frac{1}{2}} = \sum_{n=0}^{\infty} t^n P_n(u) \tag{18.32}$$

Normalisation can be achieved via:

$$I(s,t) = \int_{-1}^{1} du [1+s^2-2us]^{-\frac{1}{2}} [1+t^2-2ut]^{-\frac{1}{2}} = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} s^n t^m \int_{-1}^{1} du P_n(u) P_m(u).$$

$$\begin{aligned} I(s,t) &= \frac{1}{2\sqrt{st}} \int_{-1}^{1} du \left[ \frac{1}{2} \left( s + \frac{1}{s} \right) - u \right]^{-\frac{1}{2}} \left[ \frac{1}{2} \left( t + \frac{1}{t} \right) - u \right]^{-\frac{1}{2}} \\ &= A \int_{-1}^{1} \frac{du}{[(a-u)(b-u)]^{\frac{1}{2}}} \end{aligned} \tag{18.33}$$

where $A = \frac{1}{2\sqrt{st}}$ , $a = \frac{1}{2}\left(s + \frac{1}{s}\right)$ and $b = \frac{1}{2}\left(t + \frac{1}{t}\right)$. The integrand can be easily rewritten as:

$$I(s,t) = A \int_{-1}^{1} du \, \frac{\dfrac{1}{[a-u]^{\frac{1}{2}}} + \dfrac{1}{[b-u]^{\frac{1}{2}}}}{[a-u]^{\frac{1}{2}} + [b-u]^{\frac{1}{2}}} \tag{18.34}$$

Put $U = [a-u]^{\frac{1}{2}} + [b-u]^{\frac{1}{2}}$ then $dU = -\frac{1}{2}\left[[a-u]^{-\frac{1}{2}} + [b-u]^{-\frac{1}{2}}\right] du$. So the integral becomes

$$\begin{aligned} I(s,t) &= 2A \int_{[a-1]^{\frac{1}{2}}+[b-1]^{\frac{1}{2}}}^{[a+1]^{\frac{1}{2}}+[b+1]^{\frac{1}{2}}} \frac{dU}{U} \\ &= \frac{1}{\sqrt{st}} \Big[\ln U\Big]_{[a-1]^{\frac{1}{2}}+[b-1]^{\frac{1}{2}}}^{[a+1]^{\frac{1}{2}}+[b+1]^{\frac{1}{2}}} \\ &= \frac{1}{\sqrt{st}} \ln\left(\frac{[a+1]^{\frac{1}{2}} + [b+1]^{\frac{1}{2}}}{[a-1]^{\frac{1}{2}} + [b-1]^{\frac{1}{2}}}\right) \end{aligned} \tag{18.35}$$

Consider the individual terms within the logarithm:

$$[a+1]^{\frac{1}{2}} = \left[\frac{1}{2}\left(s + \frac{1}{s}\right) + 1\right]^{\frac{1}{2}} = \frac{1}{\sqrt{2s}}\left[\left(s^2 + 2s + 1\right)\right]^{\frac{1}{2}} = \frac{1}{\sqrt{2s}}\left[(s+1)^2\right]^{\frac{1}{2}} = \frac{1}{\sqrt{2}}(\sqrt{s} + \frac{1}{\sqrt{s}}),$$

$$[b+1]^{\frac{1}{2}} = \frac{1}{\sqrt{2}}(\sqrt{t} + \frac{1}{\sqrt{t}}), \qquad [a-1]^{\frac{1}{2}} = \frac{1}{\sqrt{2}}(\frac{1}{\sqrt{s}} - \sqrt{s}), \qquad [b-1]^{\frac{1}{2}} = \frac{1}{\sqrt{2}}(\frac{1}{\sqrt{t}} - \sqrt{t})$$

so the last term in (18.35) can be written

$$\begin{aligned} I(s,t) &= \frac{1}{\sqrt{st}} \ln \frac{\sqrt{s} + \frac{1}{\sqrt{s}} + \sqrt{t} + \frac{1}{\sqrt{t}}}{\frac{1}{\sqrt{s}} - \sqrt{s} + \frac{1}{\sqrt{t}} - \sqrt{t}} \\ &= \frac{1}{\sqrt{st}} \ln \frac{\sqrt{s} + \sqrt{t} + s\sqrt{t} + t\sqrt{s}}{\sqrt{s} + \sqrt{t} - s\sqrt{t} - t\sqrt{s}} \\ &= \frac{1}{\sqrt{st}} \ln \frac{\sqrt{s} + \sqrt{t} + \sqrt{st}(\sqrt{s} + \sqrt{t})}{\sqrt{s} + \sqrt{t} - \sqrt{st}(\sqrt{s} + \sqrt{t})} \\ &= \frac{1}{\sqrt{st}} \ln \frac{1 + \sqrt{st}}{1 - \sqrt{st}} \end{aligned} \tag{18.36}$$

where in the second line on the RHS we have multiplied top and bottom inside the logarithm by $\sqrt{st}$. This can be turned into a Taylor expansion:

$$
\begin{aligned}
I(s,t) &= \frac{1}{\sqrt{st}}\ln\frac{1+\sqrt{st}}{1-\sqrt{st}} = \frac{1}{\sqrt{st}}\left[\ln(1+\sqrt{st})-\ln(1-\sqrt{st})\right] \\
&= \frac{1}{\sqrt{st}}\left[\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}(\sqrt{st})^n+\sum_{n=1}^{\infty}\frac{1}{n}(\sqrt{st})^n\right] \\
&= \frac{1}{\sqrt{st}}\left[\sum_{n=1}^{\infty}\frac{1+(-1)^{n+1}}{n}(\sqrt{st})^n\right] \\
&= 2+\frac{2}{3}(st)+\frac{2}{5}(st)^2+\frac{2}{7}(st)^3+ \\
&= \sum_{m=0}^{\infty}\frac{2[st]^m}{1+2m}
\end{aligned}
\tag{18.37}
$$

and so:

$$
\int_{-1}^{1} duP_n(u)P_m(u) = \delta_{nm}\frac{2}{1+2n}. \tag{18.38}
$$

## 18.4 Generating function for Chebyshev Polyinomials

We can derive a generating function from (12.27) by introducing the dummy variable $t$ and noting

$$
\left(\frac{\partial}{\partial t}\right)^n e^{(x\pm\sqrt{x^2-1})t}\bigg|_{t=0} = (x\pm\sqrt{x^2-1})^n,
$$

we immediatly see that a generating function for Chebyshev polynomials is

$$
\begin{aligned}
\sum_{n=0}^{\infty}\frac{t^n}{n!}T_n(x) &= \frac{1}{2}\left(e^{(x+\sqrt{x^2-1})t}+e^{(x-\sqrt{x^2-1})t}\right) \\
&= e^{tx}\cos(t\sqrt{1-x^2}).
\end{aligned}
\tag{18.39}
$$

Another generating function can be derived as follows:

Assume $|t| < 1$ and write

$$\sum_{n=0}^{\infty} (te^{i\theta})^n = \frac{1}{1 - te^{i\theta}}$$

By taking the real part of both side we get

$$\sum_{n=0}^{\infty} t^n \cos n\theta = Re\left[\frac{1}{(1 - t\cos\theta) + it\sin\theta}\right] = \frac{1 - t\cos\theta}{1 - 2t\cos\theta + t^2}$$

and so we have a generating function for $T_n(x)$:

$$\frac{1 - tx}{1 - 2tx + t^2} = \sum_{n=0}^{\infty} t^n T_n(x). \tag{18.40}$$

### 18.4.1 Orthonormailty from genrating function

$$\begin{aligned} \int_{-1}^{1} \frac{dx}{[1 - x^2]^{\frac{1}{2}}} \frac{1 - sx}{1 - 2sx + s^2} \frac{1 - tx}{1 - 2tx + t^2} &= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} s^m t^n T_m(x) T_n(x) \\ = & \end{aligned} \tag{18.41}$$

### 18.4.2 Explicit Expression from the Generating Function

$$\begin{aligned} \frac{1 - tx}{1 - 2tx + t^2} &= (1 - tx)(1 + t^2 - 2xt)^{-1} \\ &= (1 - tx)[1 + t(2x - t) + t^2(2x - t)^2 + t^3(2x - t)^3 + \dots] \\ &= \sum_{k=0}^{\infty} t^n T_n(x) \end{aligned} \tag{18.42}$$

We need the binomial expansion again:

$$(2x - t)^m = \sum_{q=0}^{m} \frac{m!}{q!(m - q)!} (-t)^q (2x)^{m-q}$$

The coefficient of $t^n$ comes from the term $t^n(2x - t)^n$ and those below it. ($m = n$ and $q = 0$)

$$(2x)^n$$

and from $-txt^{n-1}(2x-t)^{n-1}$ ($m=n-1$ and $q=0$)

$$(-x)(2x)^{n-1}$$

and from $t^{n-1}(2x-t)^{n-1}$ ($m=n-1$ and $q=1$)

$$\frac{(n-1)!}{1!(n-2)!}(-1)(2x)^{n-2}$$

and from $-txt^{n-2}(2x-t)^{n-2}$ ($m=n-2$ and $q=1$)

$$(-x)\frac{(n-2)!}{1!(n-3)!}(-1)(2x)^{n-3}.$$

From the general term $t^{n-k}(2x-t)^{n-k}$ ($m=n-k$ and $q=k$)

$$\frac{(n-k)!}{k!(n-2k)!}(-1)^k(2x)^{n-2k}$$

and from the general term $-txt^{n-k-1}(2x-t)^{n-k-1}$ ($m=n-k-1$ and $q=k$)

$$(-x)\frac{(n-k-1)!}{k!(n-2k-1)!}(-1)^k(2x)^{n-1-2k}$$

Putting it together

$$\begin{aligned}
& \frac{(n-k)!}{k!(n-2k)!}(-1)^k(2x)^{n-2k}+(-x)\frac{(n-k-1)!}{k!(n-2k-1)!}(-1)^k(2x)^{n-1-2k} \\
= \;& (-1)^k\left[\frac{(n-k)!}{k!(n-2k)!}-\frac{1}{2}\frac{(n-k-1)!}{k!(n-2k-1)!}\right](2x)^{n-2k} \\
= \;& (-1)^k\frac{(n-k-1)!}{k!(n-2k)!}\left[(n-k)-\frac{1}{2}(n-2k)\right](2x)^{n-2k} \\
= \;& \frac{n}{2}(-1)^k\frac{(n-k-1)!}{k!(n-2k)!}(2x)^{n-2k} \qquad (18.43)
\end{aligned}$$

So that

$$T_n(x) = \frac{n}{2} \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k \frac{(n-k-1)!}{k!(n-2k)!} (2x)^{n-2k} \tag{18.44}$$

# Chapter 19

# Quantum Mechanics: Summary

The proposed method of solution involves five steps:

(1) Rescale the lengths and energy to simplify the problem.

(2) Use WKB or guess the asymptotic behaviour, which amounts to the problem.

(3) Extract the asymptotic behaviour.

(4) Search for a series solution. Truncation leads to eigenvalues.

(5) Normalisation. The generating function will usually help if it is known.

## 19.1 Example $\hat{H} = -\frac{\hbar^2}{2m} - \frac{V}{\cosh^2(x/\xi)}$

A quantum mechanics problem is that of a particle bound by a '$sech^2$' potential:

$$\hat{H} = -\frac{\hbar^2}{2m} - \frac{V}{\cosh^2(x/\xi)} \tag{19.1}$$

in one-dimension, controlled by the obvious inner-product:

$$\int_{-\infty}^{\infty} dx \psi_1^*(x)\psi_1(x) \tag{19.2}$$

Solve.

We want to use our five step proces:

(1) By scaling the length and energy, we can extract out $\xi$ and $-\frac{\hbar^2}{2m}$:

$$x = \xi z$$

$$E = \frac{\hbar^2}{2m\xi^2}\epsilon$$

$$V = \frac{\hbar^2}{2m\xi^2}\nu$$

we are led to:

$$-\frac{d^2}{dz^2} - \frac{\nu}{cosh^2 z} = \epsilon \tag{19.3}$$

This problem requires a 'cunning substitution', which is a particular to the case in point:

$$u = tanhz \qquad \frac{du}{dz} = 1 - tanh^2 z = 1 - u^2 \tag{19.4}$$

$$\frac{d}{dz} = \frac{du}{dz}\frac{d}{du} = (1-u^2)\frac{d}{du}$$

$$\frac{d^2}{dz^2} = (1-u^2)\frac{d}{du}(1-u^2)\frac{d}{du}$$

and hence (19.3) becomes:

$$-(1-u^2)^2\frac{d^2}{du^2} + 2u(1-u^2)\frac{d}{du} - \nu(1-u^2) = \epsilon$$

or

$$(1-u^2)\frac{d^2}{du^2} - 2u\frac{d}{du} + \nu + \frac{\epsilon}{1-u^2} = 0 \tag{19.5}$$

(2) The asymptotics is controlled by $\psi \sim (1-u^2)^\alpha$

$$\frac{d\psi}{du} \sim -2\alpha(1-u^2)^{\alpha-1}u$$

$$\begin{aligned}
\frac{d}{du}\left[(1-u^2)\frac{d}{du}\right]\psi &= \frac{d}{du}\left[-2\alpha(1-u^2)^{\alpha}u\right] \\
&= 4\alpha^2u^2(1-u^2)^{\alpha-1} - 2\alpha(1-u^2)^{\alpha} \\
&= 4\alpha^2(1-u^2)^{\alpha-1}[1-(1-u^2)] - 2\alpha(1-u^2)^{\alpha} \\
&= 4\alpha^2(1-u^2)^{\alpha-1} - 2\alpha(2\alpha+1)(1-u^2)^{\alpha} \qquad (19.6)
\end{aligned}$$

so $4\alpha^2+\epsilon=0$ and $\epsilon<0$ and we choose to use $\epsilon=-m^2$ and then $m=2\alpha$ constitutes the asymptotics.

(3) Extract out the asymptotics using;

$$\psi(u) = (1-u^2)^{m/2}P(u) \qquad (19.7)$$

$$\frac{d\psi}{du} = (1-u^2)^{m/2}\frac{dP}{du} - mu(1-u^2)^{(m-2)/2}P$$

$$\begin{aligned}
\frac{d^2\psi}{du^2} &= (1-u^2)^{m/2}\frac{d^2P}{du^2} - 2mu(1-u^2)^{(m-2)/2}\frac{dP}{du} \\
&+ \left[m(m-2)u^2(1-u^2)^{(m-4)/2} - m(1-u^2)^{(m-2)/2}\right]P
\end{aligned}$$

and so

$$(1-u^2)\frac{d^2\psi}{du^2} - 2u\frac{d\psi}{du} + [\nu + \frac{\epsilon}{1-u^2}]\psi = 0$$

becomes:

$$\begin{aligned}
&(1-u^2)\Big[(1-u^2)^{m/2}\frac{d^2P}{du^2} - 2mu(1-u^2)^{(m-2)/2}\frac{dP}{du} \\
&\quad + \left[m(m-2)u^2(1-u^2)^{(m-4)/2} - m(1-u^2)^{(m-2)/2}\right]P\Big] \\
&-2u\left[(1-u^2)^{m/2}\frac{dP}{du} - mu(1-u^2)^{(m-2)/2}P\right] + \left[\nu - \frac{m^2}{1-u^2}\right](1-u^2)^{m/2}P = 0
\end{aligned} \qquad (19.8)$$

and so:

$$
\begin{aligned}
&(1-u^2)\frac{d^2P}{du^2} - 2(m+1)u\frac{dP}{du} + \\
&+ \left[m(m-2)u^2(1-u^2)^{-1} - m\right] P \\
&+2mu^2(1-u^2)^{-1}P + \left[\nu - \frac{m^2}{1-u^2}\right] P = 0
\end{aligned}
$$

or

$$
(1-u^2)\frac{d^2P}{du^2} - 2(m+1)u\frac{dP}{du} + [\nu - m^2 - m]P = 0. \tag{19.9}
$$

(4) Two types of scaling for the series solution, and:

$$
\frac{d^2P}{du^2} = u^2\frac{d^2P}{du^2} + 2(m+1)u\frac{dP}{du} + [m^2 + m - \nu]P
$$

$$
\frac{d^2P}{du^2} = \sum_{n=0}^{\infty} a_n(n+\sigma)(n+\sigma-1)u^{n+\sigma-2} = \sum_{n=-2}^{\infty} a_{n+2}(n+\sigma+2)(n+\sigma+1)u^{n+\sigma}
$$

$$
\begin{aligned}
&u^2\frac{d^2P}{du^2} + 2(m+1)u\frac{dP}{du} + [m^2 + m - \nu]P \\
&= \sum_{n=0}^{\infty} a_n[(n+\sigma)(n+\sigma-1) + 2(m+1)(n+\sigma) + m(m+1) - \nu]u^{n+\sigma}
\end{aligned}
$$

so $a_0\sigma(\sigma-1) = 0$ and $a_1(\sigma+1)\sigma = 0$ and $\sigma = 0$.

The final equations become:

$$
\frac{d^2P}{du^2} = \sum_{n=-2}^{\infty} a_{n+2}(n+2)(n+1)u^n
$$

$$
\begin{aligned}
&u^2\frac{d^2P}{du^2} + 2(m+1)u\frac{dP}{du} + [m^2 + m - \nu]P \\
&= \sum_{n=0}^{\infty} a_n[n(n-1) + 2(m+1)n + m(m+1) - \nu]u^n
\end{aligned}
$$

from which we can deduce the eigenvalues and eigenvectors:

$$(n+2)(n+1)a_{n+2} = a_n[n(n+2m+1)+m(m+1)-\nu] = a_n\left[(n+m+\frac{1}{2})^2 - \frac{1}{4} - \nu\right]$$

and the eigenvalues are found from the condition

$$(N+m+\frac{1}{2})^2 - \frac{1}{4} - \nu = 0$$

and so satisfy:

$$m = \left[\frac{1}{4}+\nu\right]^{1/2} - \frac{1}{2} - N \geq 0$$

for a positive integer $N$.

There is always at least one solution, $N=0$, and if we set $\nu = l(l+1)$, then $m = l-N \geq 0$ and the integer part of $l+1$ counts the number of bound states.

Note that the weight function is $(1-u^2)^{m-1}$, since $du = (1-u^2)dz$ gives an additional factor of $1/(1-u^2)$ when dealing with a non-linear transformation. $P(u) \mapsto$ constant as $u \mapsto \pm 1$ is *not* normalisable, for $\epsilon = 0 = m$, and these solutions are relevant for the motion of so-called 'solitons'.

A few solutions are:

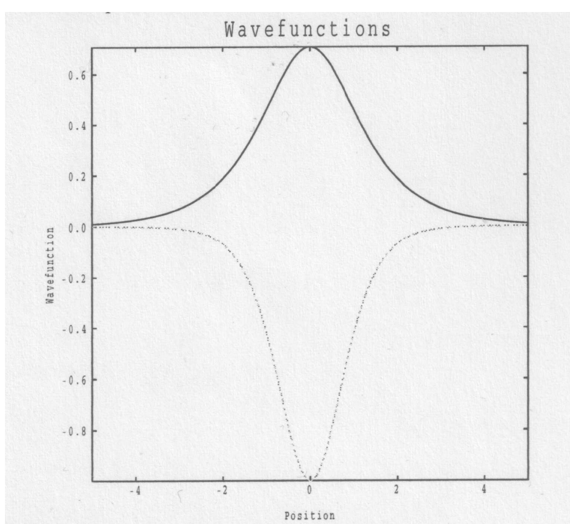



Figure 19.1: when $\nu = 2$ and the second bound state is about to appear:

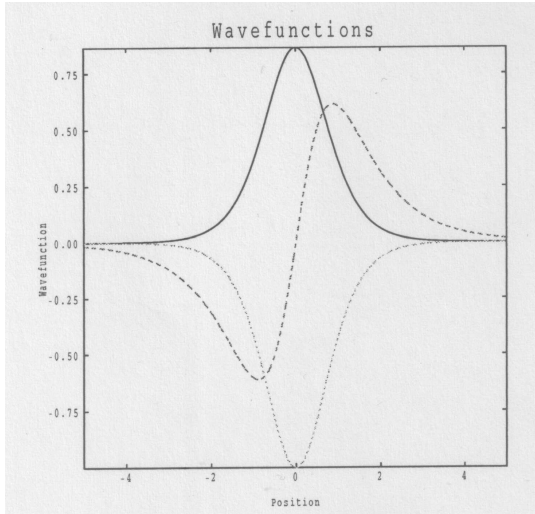



Figure 19.2: when $\nu = 6$ and the third bound state is about to appear:

## 19.2 Example $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - U \exp\left[\frac{x}{\xi}\right] + V \exp\left[\frac{2x}{\xi}\right]$

A quantum mechanics problem is that of a particle bound to a 'surface' potential:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - U \exp\left[\frac{x}{\xi}\right] + V \exp\left[\frac{2x}{\xi}\right] \tag{19.10}$$

in one-dimension, controlled by the obvious inner-product:

$$\int_{-\infty}^{\infty} dx \psi_1^*(x)\psi_1(x) \tag{19.11}$$

Solve.

We want to use our five step process:

(1)

In this problem there is no natural origin, and so we are free to choose the origin as well as rescale the length and energy:

$$x \mapsto \xi(x + \alpha) \qquad E \mapsto \beta\epsilon.$$

This leads to:

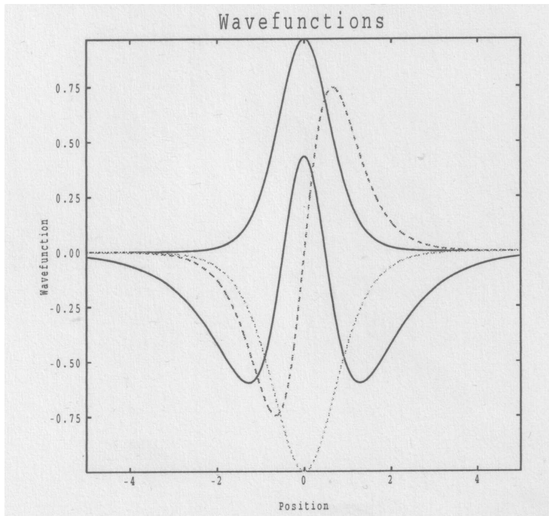



Figure 19.3: when $\nu = 12$ and the fourth bound state is about to appear.

$$\hat{H} - E = -\frac{\hbar^2}{2m\xi^2}\frac{d^2}{dz^2} - U\exp\left(\alpha + z\right) + V\exp\left(2\alpha + 2z\right) - \beta\epsilon$$

and with the choice:

$$\beta = \frac{\hbar^2}{2m\xi^2} \qquad U\exp(\alpha) = 2\beta\nu^2 \qquad V\exp(2\alpha) = \beta\nu^2$$

i.e.

$$\exp(\alpha) = \frac{U}{2V} \qquad \nu^2 = \frac{U^2 m\xi^2}{2V\hbar^2}$$

we arrive at the rescaled problem:

$$\beta^{-1}[\hat{H} - E] \mapsto -\frac{d^2}{dz^2} - 2\nu^2\exp(z) + \nu^2\exp(2z) - \epsilon$$

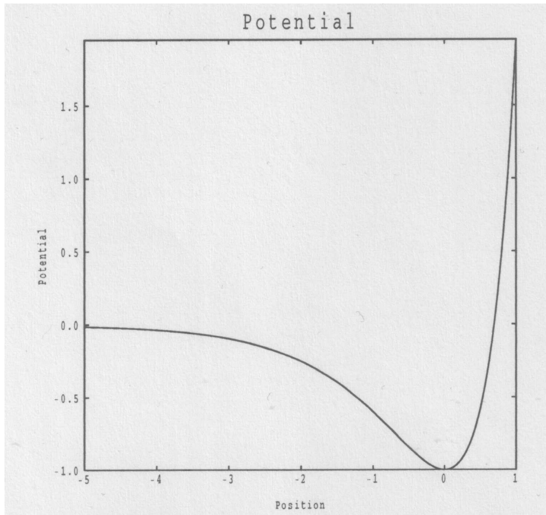
where we have chosen the minimum of the potential to be the origin.

Unfortunately, this problem is not immediately accessible to our techniques and require a non-linear transformation $u = \exp(z)$ to simplify it to:

$$-u\frac{d}{du}u\frac{d}{du} - 2\nu^2 u + \nu^2 u^2 - \epsilon$$

and is clearly much like that which would be expected close to an attractive surface.

The corresponding potential for the case $\nu = 1$ is:




(2) The asymptotics may be deduced with WKB:

$$\frac{d^2\psi}{du^2} \mapsto \left[\frac{d\phi}{du}\right]^2$$

and hence

$$\left[\frac{d\phi}{du}\right]^2 - \frac{1}{u}\frac{d\phi}{du} - \frac{2\nu^2}{u} + \nu^2 - \frac{\epsilon}{u^2} = 0$$

which provides, in the limit $u \mapsto \infty$:

$$\phi \sim \pm\nu u \quad \textit{implies} \quad \psi \sim \exp\left[-\nu u\right]$$

(3) The asymptotics may be extracted employing $\psi(u) = \exp(-\nu u)P(u)$:

$$\frac{d\psi}{du} = e^{-\nu u}\left[\frac{dP}{du} - \nu P\right]$$

$$\frac{d^2\psi}{du^2} = e^{-\nu u}\left[\frac{d^2P}{du^2} - 2\nu\frac{dP}{du} + \nu^2 P\right]$$

and so:

$$-u^2\frac{d^2\psi}{du^2} - u\frac{d\psi}{du} - 2\nu^2 u\psi + \nu^2 u^2\psi - \epsilon\psi = -e^{-\nu u}u^2\left[\frac{d^2P}{du^2} - 2\nu\frac{dP}{du} + \nu^2 P\right]$$
$$-e^{-\nu u}u\left[\frac{dP}{du} - \nu P\right] + e^{-\nu u}\left[-2\nu^2 u + \nu^2 u^2 - \epsilon\right]P = 0 \qquad (19.12)$$

or

$$u^2\frac{d^2P}{du^2} + (u - 2\nu u^2)\frac{dP}{du} + (\epsilon - \nu u + 2\nu^2 u)P = 0$$

(4) Although we could (and perhaps should) extract the asymptotic properties as $u \mapsto 0$, we elect to allow the series solution to do it for us via the parameter $\sigma$. There are two types of scaling in the system:

$$\begin{aligned} u^2\frac{d^2P}{du^2} + u\frac{dP}{du} + \epsilon P &= \sum_{n=0}^{\infty}[(n+\sigma)(n+\sigma-1) + (n+\sigma) + \epsilon]a_n u^{n+\sigma} \\ &\mapsto \sum_{n=0}^{\infty}\left((n+\sigma)^2 + \epsilon\right)a_n u^{n+\sigma} \end{aligned}$$

$$\begin{aligned} 2\nu u^2\frac{dP}{du} + (\nu - 2\nu^2)uP &= \sum_{n=0}^{\infty}[2\nu(n+\sigma) + (\nu - 2\nu^2)]a_n u^{n+1+\sigma} \\ &\mapsto \sum_{n=0}^{\infty} 2\nu\left(n + \sigma + \frac{1}{2} - \nu\right)a_n u^{n+1+\sigma}. \end{aligned} \qquad (19.13)$$

Separating them to opposite sides of the equation:

$$u^2\frac{d^2P}{du^2} + u\frac{dP}{du} + \epsilon P = 2\nu u^2\frac{dP}{du} + (\nu - 2\nu^2)$$

we then substitute in the series expansions:

$$\sum_{n=0}^{\infty}\left((n+\sigma)^2 + \epsilon\right)a_n u^{n+\sigma} = \sum_{n=0}^{\infty} 2\nu\left(n + \sigma + \frac{1}{2} - \nu\right)a_n u^{n+1+\sigma}.$$

The series on the LHs has an additional term at the start which requires to vanish:

$$\left(\sigma^2+\epsilon\right)a_0=0$$

ensuring that $\epsilon=-\sigma^2$ and then we have:

$$\sum_{n=0}^{\infty}\left((n+1+\sigma)^2-\sigma^2\right)a_{n+1}u^{n+1+\sigma}=\sum_{n=0}^{\infty}2\nu\left(n+\sigma+\frac{1}{2}-\nu\right)a_n u^{n+1+\sigma}.$$

as all of the different coefficients of $u$ must be equal, we have:

$$\left((n+1+\sigma)^2-\sigma^2\right)a_{n+1}=2\nu\left(n+\sigma+\frac{1}{2}-\nu\right)a_n$$

which gives us the recurrence relationship:

$$a_{n+1}=2\nu\frac{\left(n+\sigma+\frac{1}{2}-\nu\right)}{(n+1)(n+1+2\sigma)}a_n.$$

The spectrum is attained when this recurrence relationship terminates:

$$\sigma=\nu-\frac{1}{2}-N>0\qquad\text{implies}\qquad\epsilon=-\left(\nu-\frac{1}{2}-N\right)^2$$

It is straightforward to solve this relationship for the first few solutions:

$$P_0(u)=u^\sigma\qquad N=\nu-\sigma-\frac{1}{2}=0$$

$$P_1(u)=u^\sigma\left(1-\frac{\nu u}{\nu-1}\right)\qquad N=\nu-\sigma-\frac{1}{2}=1$$

$$P_2(u)=u^\sigma\left(1-\frac{\nu u}{\nu-1}+\frac{2\nu^2u^2}{(\nu-2)(2\nu-3)}\right)\qquad N=\nu-\sigma-\frac{1}{2}=2$$

as

$$a_2=2\nu\frac{\left(1+\sigma+\frac{1}{2}-\nu\right)}{2(2+2\sigma)}a_1=2\nu\frac{-1}{2(-3+2\nu)}(-\frac{\nu}{\nu-1})$$

and in terms of the original coordinate ($\psi(z)=\exp(-\nu\exp(z))P(\exp(z))$):

$$\psi_0(z) = \exp\left[-\nu e^z + z(\nu - \frac{1}{2})\right] \qquad N = \nu - \sigma - \frac{1}{2} = 0$$

$$\psi_1(z) = \exp\left[-\nu e^z + z(\nu - \frac{3}{2})\right]\left(1 - \frac{\nu e^z}{\nu - 1}\right) \qquad N = \nu - \sigma - \frac{1}{2} = 1$$

$$\psi_2(z) = \exp\left[-\nu e^z + z(\nu - \frac{5}{2})\right]\left(1 - \frac{\nu e^z}{\nu - 1} + \frac{2\nu^2 e^{2z}}{(\nu-2)(2\nu-3)}\right) \qquad N = \nu - \sigma - \frac{1}{2} = 2$$

**Case:** $\nu = 1$

The potential is:

$$-2\exp(z) + \exp(2z)$$

and the recurrence relationship is:

$$a_{n+1} = 2\frac{\left(n + \sigma - \frac{1}{2}\right)}{(n+1)(n+1+2\sigma)}a_n.$$

The spectrum is attained when this recurrence relationship terminates:

$$\sigma = \frac{1}{2} - N > 0 \qquad \text{implies} \qquad \epsilon = -\left(\frac{1}{2} - N\right)^2$$

$N = 0:$

Then $a_0 = 1$ and $a_1 = 0$ $(\sigma = 1/2)$

$$P_0(u) = u^{1/2} \qquad \psi_0(z) = \exp\left[-e^z + z\frac{1}{2}\right]$$

**Case:** $\nu = 2$

The potential is:

$$-8\exp(z) + 4\exp(2z)$$

and the recurrence relationship is:

$$a_{n+1} = 4 \frac{\left(n + \sigma - \frac{3}{2}\right)}{(n+1)(n+1+2\sigma)} a_n.$$

The spectrum is attained when this recurrence relationship terminates:

$$\sigma = \frac{3}{2} - N > 0 \qquad \text{implies} \qquad \epsilon = -\left(\frac{3}{2} - N\right)^2$$

$N = 0:$

Then $a_0 = 1$ and $a_1 = 0$ $(\sigma = 3/2)$

$$P_0(u) = u^{3/2} \qquad \psi_0(z) = \exp\left[-2e^z + z\frac{3}{2}\right]$$

$N = 1:$

Then $a_0 = 1$, $a_1 \neq 0$ and $a_2 = 0$ $(\sigma = 1/2)$

$$P_1(u) = u^{1/2}\,(1 - 2u) \qquad \psi_1(z) = \exp\left[-2e^z + z\frac{1}{2}\right](1 - 2e^z)$$

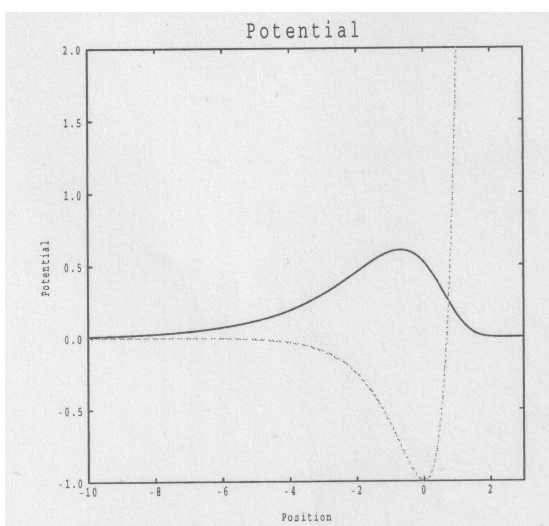



Figure 19.4: The case $\nu = 1$ with its single bound state is depicted

and

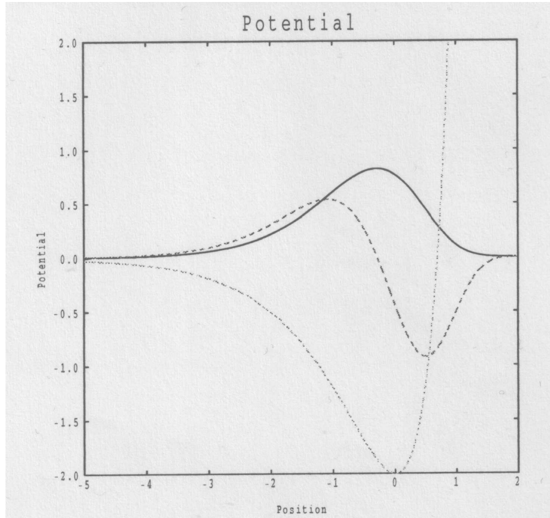



Figure 19.5: the case of $\nu = 2$ with ts two bounds states is also depicted

## 19.3 Example $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{V}{\sin^2(x/\xi)}$

A quantum mechanics problem is that of a particle bound to a '*cosec*$^2$' potential:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{V}{\sin^2(x/\xi)} \tag{19.14}$$

in one-dimension, controlled by the obvious inner-product:

$$\int_0^{\xi\pi} dx \psi_1^*(x)\psi_1(x) \tag{19.15}$$

where the particle is restricted to the region $x \in (0, \xi\pi)$. Solve.

We want to use our five step process:

(1) By scaling the length and energy, we can extract out $\xi$ and $-\frac{\hbar^2}{2m}$:

$$x = \xi z$$
$$E = \frac{\hbar^2}{2m\xi^2}\epsilon$$
$$V = \frac{\hbar^2}{2m\xi^2}\nu(\nu - 1)$$

we are led to:

$$-\frac{d^2}{dz^2} + \frac{\nu(\nu-1)}{\sin^2 z} = \epsilon.$$

This problemnow requires a 'cunning substitution', which is aprticular to the case in point:

$$\begin{aligned} u = \cos z \quad \frac{du}{dz} &= -\sin z = -\left[1-u^2\right]^{\frac{1}{2}} \\ \frac{d}{dz} &= \frac{du}{dz}\frac{d}{du} = -\left[1-u^2\right]^{\frac{1}{2}}\frac{d}{du} \\ \frac{d^2}{dz^2} &= \left[1-u^2\right]\frac{d}{du}\left[1-u^2\right]\frac{d}{du} \end{aligned}$$

and hence:

$$-(1-u^2)\frac{d^2}{du^2} + u\frac{d}{du} - \frac{\nu(\nu-1)}{(1-u^2)} = \epsilon.$$

(2) The asymptotics is controlled by $\psi \sim (1-u^2)^\alpha$

$$\frac{d\psi}{du} \sim -2\alpha(1-u^2)^{\alpha-1}u$$

$$\begin{aligned} \left[1-u^2\right]^{\frac{1}{2}}\frac{d}{du}\left[\left[1-u^2\right]^{\frac{1}{2}}\frac{d}{du}\right]\psi &= 2\alpha(2\alpha-1)u^2(1-u^2)^{\alpha-1} - 2\alpha(1-u^2)^\alpha \\ &= 2\alpha(2\alpha-1)(1-u^2)^{\alpha-1} - 4\alpha^2(1-u^2)^\alpha \end{aligned}$$

so $2\alpha(2\alpha-1) = \nu(\nu-1)$ and $2\alpha = \nu$ or $2\alpha = 1-\nu$. We choose to use $\nu > \frac{1}{2}$ and $2\alpha = \nu$ which is required by the form of the potential.

(3) Extract out the asymptotics using:

$$\begin{aligned} \psi(u) &= (1-u^2)^{\nu/2}P(u) \\ \frac{d\psi}{du} &= (1-u^2)^{\nu/2}\frac{dP}{du} - \nu u(1-u^2)^{(\nu-2)/2}P \end{aligned}$$

$$\begin{aligned} \frac{d^2\psi}{du^2} &= (1-u^2)^{\nu/2}\frac{d^2P}{du^2} - 2\nu u(1-u^2)^{(\nu-2)/2}\frac{dP}{du} \\ &+ \left[\nu(\nu-2)u^2(1-u^2)^{(\nu-4)/2} - \nu(1-u^2)^{(\nu-2)/2}\right]P \end{aligned}$$

and so

$$(1-u^2)\frac{d^2P}{du^2} - (2\nu+1)u\frac{dP}{du} + [\epsilon - \nu^2]P = 0$$

(4) Two types of scaling for the series solution, and:

$$\frac{d^2P}{du^2} = u^2\frac{d^2P}{du^2} + (2\nu+1)u\frac{dP}{du} + [\nu^2 - \epsilon]P$$

$$\frac{d^2P}{du^2} = \sum_{n=0}^{\infty} a_n(n+\sigma)(n+\sigma-1)u^{n+\sigma-2} = \sum_{n=-2}^{\infty} a_n(n+\sigma+2)(n+\sigma+1)u^{n+\sigma}$$

$$\begin{aligned} & u^2\frac{d^2P}{du^2} + (2\nu+1)u\frac{dP}{du} + [\nu^2 - \epsilon]P \\ = & \sum_{n=0}^{\infty} a_n[(n+\sigma)(n+\sigma-1) + (2\nu+1)(n+\sigma) + \nu^2 - \epsilon]u^{n+\sigma} \end{aligned} \tag{19.16}$$

so $a_0\sigma(\sigma-1) = 0$ and $a_1(\sigma+1)\sigma = 0$ and $\sigma = 0$.

The final equation become:

$$\frac{d^2P}{du^2} = \sum_{n=-2}^{\infty} a_{n+2}(n+2)(n+1)u^n$$

$$\begin{aligned} & u^2\frac{d^2P}{du^2} + (2\nu+1)u\frac{dP}{du} + [\nu^2 - \epsilon]P \\ = & \sum_{n=0}^{\infty} a_n[n^2 + 2n\nu + \nu^2 - \epsilon]u^n \end{aligned}$$

from which we can deduce the eigenvalues and eigenvectors:

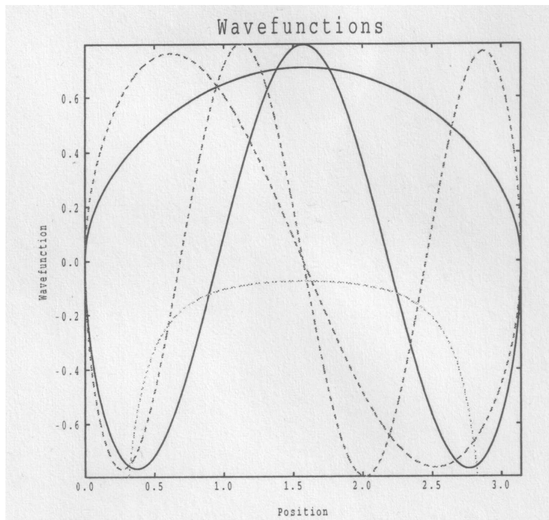
$$(n+2)(n+1)a_{n+2} = a_n[(n+\nu)^2 - \epsilon]$$

and the eigenvalues satisfy:

$$\epsilon = (N+\nu)^2$$

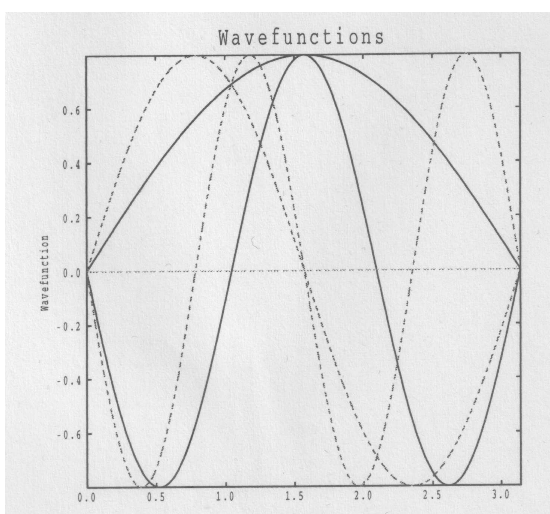
for a positive integer $N$.

There are always an infinite number of bound states, although their character varies wildly as $\nu$ is varied. When $\nu \in \left(\frac{1}{2}, 1\right)$, the potential is negative and the particle is attracted to the edge of the system although it is still repelled by the lack of space outside of its permitted region. If $\nu \leq \frac{1}{2}$ is considered, then the kinetic energy is not strong enough to stop the particle from becoming localised at the edge of the system and the whole picture breaks down. The first four wavefunctions are depicted for the case $\nu \mapsto \frac{1}{2}$:

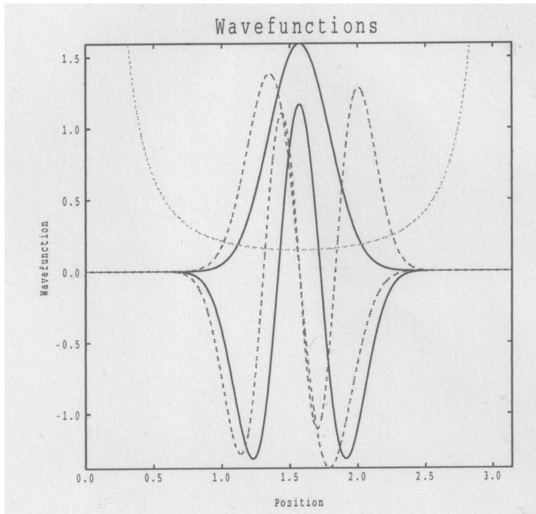



The cusp at the edge of the system is clearly indicative of the imminent breakdown to the particle becoming localised at the edge of the system.

There is a special case $\nu = 1$ where the potential vanishes and a particle in an infinite walled box remain:



The final natural limit to consider is $\nu \mapsto \infty$, where the potential becomes dominant and the kinetic energy becomes a weak perturbative addition. The particle becomes localised in the centre of theregion now, where the potential is at its smallest, and now only feels the quadratic in the Taylor's expansion about this point. The problem reduces down to that of a Harmonic Oscillator:




You may like to consider the effective inner-product:

$$\int_0^\pi dz \psi_1^*(z)\psi_2(z) \mapsto \int_{-1}^1 \frac{du}{\left[1-u^2\right]^{\frac{1}{2}}}\psi_1^*(u)\psi_2(u) = \int_{-1}^1 du \left[1-u^2\right]^{\nu-\frac{1}{2}} P_1^*(u)P_2(u)$$

which is clearly Gram-Schmidt orthogonalised by:

$$P_n^{(\nu)}(u) = \left[1-u^2\right]^{\frac{1}{2}-\nu}\left[\frac{d}{du}\right]^n \left[1-u^2\right]^{n+\nu-\frac{1}{2}} \qquad \nu > \frac{1}{2}$$

and you may like to verify using Leibnitz that these polynomials do satisfy the requisite equation:

$$(1-u^2)\frac{d^2P_n}{du^2} - (2\nu+1)u\frac{dP_n}{du} + (n^2+2\nu n)P_n = 0.$$

**Solution:**

We first note that

$$\frac{d}{du}\left[1-u^2\right]^{n+\nu-\frac{1}{2}} = -(2n+2\nu-1)u\left[1-u^2\right]^{n+\nu-1-\frac{1}{2}} \tag{19.17}$$

or

$$(1-u^2)\frac{d}{du}\left[1-u^2\right]^{n+\nu-\frac{1}{2}}+(2n+2\nu-1)u\left[1-u^2\right]^{n+\nu-\frac{1}{2}}=0. \tag{19.18}$$

and set

$$P_n'=\left[1-u^2\right]^{-(\frac{1}{2}-\nu)}P_n=\left[\frac{d}{du}\right]^n\left[1-u^2\right]^{n+\nu-\frac{1}{2}}$$

We derived in chapter 12 using (truncated) Leibnitz

$$\left(\frac{d}{du}\right)^{n+1}(uf(u))=u\left(\frac{d}{du}\right)^{n+1}f(u)+(n+1)\left(\frac{d}{du}\right)^n f(u)$$

and

$$\begin{aligned}
&\left(\frac{d}{du}\right)^{n+1}\left[(1-u^2)g(u)\right]\\
=\;&(1-u^2)\left(\frac{d}{du}\right)^{n+1}g(u)-2(n+1)u\left(\frac{d}{du}\right)^n g(u)-n(n+1)\left(\frac{d}{du}\right)^{n-1}g(u)
\end{aligned}$$

Applying $\left(\frac{d}{du}\right)^{n+1}$ to (19.18) we obtain

$$\begin{aligned}
&\left(\frac{d}{du}\right)^{n+1}\left[(1-u^2)\frac{d}{du}\left[1-u^2\right]^{n+\nu-\frac{1}{2}}+(2n+2\nu-1)u\left[1-u^2\right]^{n+\nu-\frac{1}{2}}\right]\\
=\;&(1-u^2)\frac{d^2}{du^2}\left(\frac{d}{du}\right)^n\left[1-u^2\right]^{n+\nu-\frac{1}{2}}-2(n+1)u\frac{d}{du}\left(\frac{d}{du}\right)^n\left[1-u^2\right]^{n+\nu-\frac{1}{2}}\\
&-n(n+1)\left(\frac{d}{du}\right)^n\left[1-u^2\right]^{n+\nu-\frac{1}{2}}\\
&+(2n+2\nu-1)u\frac{d}{du}\left(\frac{d}{du}\right)^n\left[1-u^2\right]^{n+\nu-\frac{1}{2}}+(2n+2\nu-1)(n+1)\left(\frac{d}{du}\right)^n\left[1-u^2\right]^{n+\nu-\frac{1}{2}}\\
=\;&(1-u^2)\frac{d^2}{du^2}P_n'-2(n+1)u\frac{d}{du}P_n'-n(n+1)P_n'+(2n+2\nu-1)u\frac{d}{du}P_n'\\
&+(2n+2\nu-1)(n+1)P_n'\\
=\;&(1-u^2)\frac{d^2}{du^2}P_n'-(3-2\nu)u\frac{d}{du}P_n'+(n+2\nu-1)(n+1)P_n'=0. \qquad (19.19)
\end{aligned}$$

Using Leibnitz

$$
\begin{aligned}
\frac{d^2}{du^2}([1-u^2]^{\nu-\frac{1}{2}}P_n) &= [1-u^2]^{\nu-\frac{1}{2}}\frac{d^2P_n}{du^2} + 2\frac{d}{du}[1-u^2]^{\nu-\frac{1}{2}}\frac{dP_n}{du} + \frac{d^2}{du^2}[1-u^2]^{\nu-\frac{1}{2}}P_n \\
&= [1-u^2]^{\nu-\frac{1}{2}}\frac{d^2P_n}{du^2} + 2(1-2\nu)u[1-u^2]^{\nu-\frac{3}{2}}\frac{dP_n}{du} \\
&\quad + (1-2\nu)(1-2\nu u^2+2u^2)[1-u^2]^{\nu-\frac{5}{2}}P_n
\end{aligned}
$$

and

$$
\frac{d}{du}([1-u^2]^{\nu-\frac{1}{2}}P_n) = [1-u^2]^{\nu-\frac{1}{2}}\frac{dP_n}{du} + u(1-2\nu)[1-u^2]^{\nu-\frac{3}{2}}P_n
$$

Substituting these into the last line of (19.19) and multiplying by $[1-u^2]^{\nu-\frac{1}{2}}$

$$
\begin{aligned}
& (1-u^2)\left(\frac{d^2P_n}{du^2} + 2(1-2\nu)u\frac{1}{1-u^2}\frac{dP_n}{du} + (1-2\nu)\frac{1-2\nu u^2+2u^2}{(1-u^2)^2}P_n\right) \\
& -(3-2\nu)u\left(\frac{dP_n}{du} + (1-2\nu)u\frac{1}{1-u^2}P_n\right) + (n^2-1+2\nu(n+1))P_n \\
= \;& (1-u^2)\frac{d^2P_n}{du^2} + [2(1-2\nu)-(3-2\nu)]u\frac{dP_n}{du} \\
& + \left((1-2\nu)\frac{1-2\nu u^2+2u^2}{(1-u^2)} - (3-2\nu)(1-2\nu)\frac{u^2}{1-u^2} + (n^2-1+2\nu(n+1))\right)P_n \\
= \;& (1-u^2)\frac{d^2P_n}{du^2} - (2\nu+1)u\frac{dP_n}{du} \\
& + \left((1-2\nu)[\frac{1-2\nu u^2+2u^2-(3-2\nu)u^2}{(1-u^2)}] + (n^2-1+2\nu(n+1))\right)P_n \\
= \;& (1-u^2)\frac{d^2P_n}{du^2} - (2\nu+1)u\frac{dP_n}{du} + [(1-2\nu)+(n^2-1+2\nu(n+1))]P_n = 0.
\end{aligned}
$$

Simplifies to

$$
(1-u^2)\frac{d^2P_n}{du^2} - (2\nu+1)u\frac{dP_n}{du} + (n^2+2\nu n)P_n = 0.
$$

# Chapter 20

# Advanced Topics: Unbounded Operators on Hilbert Space

The mathematical definition of a Hilbert space is a complete inner product space.

The'generalised' eigenfunctions of unbounded operators aren't normalisable in the inner product.

# Chapter 21

# Advanced Topics: Rigged Hilbert Space

## 21.1 Introduction

A rigged Hilbert space - also called the Gel'fand triple: In infinite dimensional Hilbert space there can be operators that have a continuous spectrum, (the most simple example would be that of a free electron which has a continuous momentum spectrum). The corresponding eigenvectors are not normalizable, and hence cannot lie inside the Hilbert space $\mathcal{H}$, (the eigenvector of the momentum operator of a free electron is a plane wave $e^{ikx}$ , which isn't normalizable). The rigged Hilbert space approach to dealing with such operators on or a Gel'fand triple $\{\Phi, \mathcal{H}, \Phi'\}$, in which the Hilbert space $\mathcal{H}$ appears as a linear subspace $\Phi'$ which is not itself a Hilbert space. Eigenvectors associated with a continuous spectrum belong to $\Phi'$ but are no members of its subspace $\mathcal{H}$. The space $\Phi'$ is constructed as a type of dual of another vector space $\Phi$ which is a subspace of $\mathcal{H}$. Thus we have $\Phi \subset \mathcal{H} \subset \Phi'$.

# Appendix A

# The Diveregence Theroem and Stokes Theorem

## A.1 Proof of Gauss's Divergence Theorem

Say we have a closed surface $S$ that encloses a volume $V$. Separate the volume into two parts by taking a slice resulting it two closed surfaces and volumes as in fig .. The volume $V_1$ is enclosed by the closed surface $S_1$, which is made up of part of the original surface $S_1'$ and of the surface of the slice $S_{12}$. The volume $V_2$ is enclosed by $S_2$, which is made up of the rest of the original surface $S_2'$ and the surface of the slice $S_{12}$. The flux through $S_1$ is

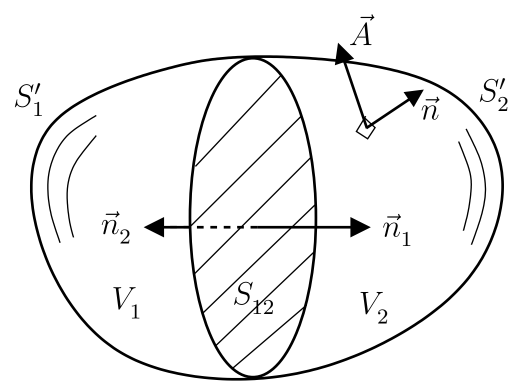



Figure A.1: .

We then have $S_1 = S_1' + S_{12}$ and $S_2 = S_2' + S_{12}$. The flux through $S_1$ can be written as the sum of two parts

$$\int_{S_1'} \vec{A} \cdot \vec{n} dS + \int_{S_{12}} \vec{A} \cdot \vec{n}_1 dS \tag{A.1}$$

and similarly for the flux through $S_2$,

$$\int_{S_2'} \vec{A} \cdot \vec{n} dS + \int_{S_{12}} \vec{A} \cdot \vec{n}_2 dS \tag{A.2}$$

As $\vec{n}_1 = -\vec{n}_2$, adding the fluxes of each of these surfaces gives

$$\int_{S_1'} \vec{A} \cdot \vec{n} dS + \int_{S_2'} \vec{A} \cdot \vec{n} dS \tag{A.3}$$

which is just to the flux through the original surface $S = S_1 + S_2$. We can subdivide the volume again and again and it will generally be true that the flux through the outer surface will be equal to the sum of the fluxes out of all the smaller interior pieces.

We now consider the special case of the flux out of a small cube.

$$\left[A_x + \frac{\partial A_x}{\partial x} dx\right] dydz - A_x dydz = \frac{\partial A_x}{\partial x} dxdydz \tag{A.4}$$

Similar contributions come from the other two pairs of faces, adding together their contributions the total flux through all faces is

$$\int_{cube} \vec{A} \cdot \vec{n} dS = \left(\frac{\partial A_1}{\partial x} + \frac{\partial A_2}{\partial y} + \frac{\partial A_3}{\partial z}\right) dxdydz \tag{A.5}$$

or

$$\int_{cube} \vec{A} \cdot \vec{n} dS = (\nabla \cdot \vec{A}) dxdydz \tag{A.6}$$

Splitting the volume $V$ enclosed by a closed surface $S$ into infintesimally small cubes, summing the LHS of the above equation gives the total flux out of the closed surface and summing over the RHS gives the volume integral

$$\int_V \nabla \cdot \vec{A} dV$$

resulting in

$$\int_S \vec{A} \cdot \vec{n} dS = \int_V \nabla \cdot \vec{A} dV \tag{A.7}$$

## A.2 Proof of Stokes' Theorem

Let us find the circulation around an infintesimal square.

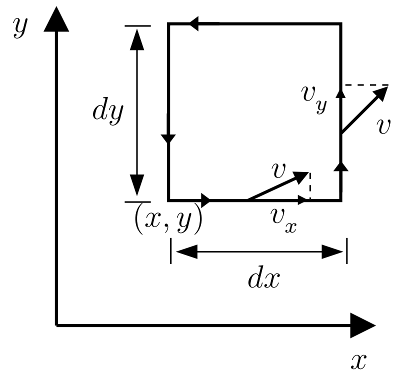



Figure A.2: Finding the circulation around an infintesimal square.

The circulation around the square is then

$$\begin{aligned}\oint \vec{v}\cdot d\vec{l} &= v_x dx + (v_y + \frac{\partial v_y}{\partial x})dy - (v_x + \frac{\partial v_x}{\partial y})dx - v_y dy \\ &= \left(\frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y}\right) dxdy \end{aligned} \tag{A.8}$$

Now say we had a collection of such squares as in fig (B.2) and wished to add up the circulation from each individual square. Interior paths are transversed in opposite directions, thus their contributions to each line integral cancel pairwise. Therefore only the outside edge contributes. This observation is an underlying principle in the proof of Stoke's theorem.

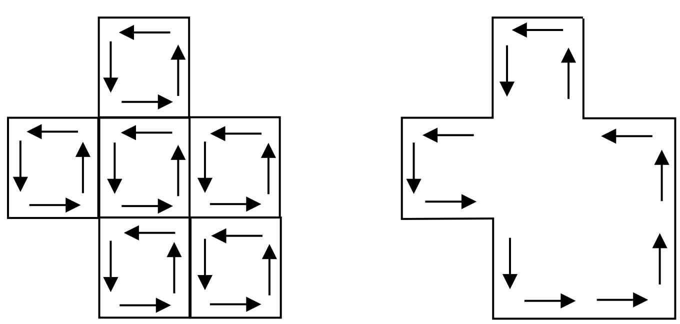


Figure A.3: When adding together the circulation of each loop the only remaing contribution to the line integral comes from the outside edge.

We can write (A.8)

$$(\nabla \times \vec{v})_z dS \tag{A.9}$$

Here the $z$-component is the normal to the surface. We can therefore write the circulation around a infintesimal square in an invariant vector form,

$$\oint_C \vec{v} \cdot d\vec{l} = (\nabla \times \vec{v}) \cdot \vec{n} dS \tag{A.10}$$

So we have that the circulation of any vector $\vec{A}$ around an infintesimal square is the component of the curl of $\vec{v}$ normal to the surface, times the area of the square. This result is independent on the orientation of the square.

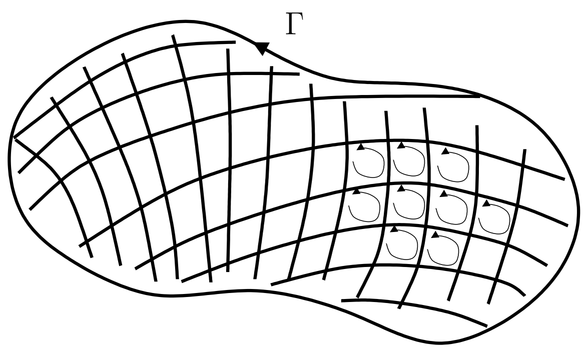



Figure A.4: We have some surface bounded by the loop Γ. The surface is divided into many small areas, each approximately a square.

Now suppose that we have a loop which is the boundary of some surface. There are of course an infinite number of surfaces that have all have this loop as their boundary. However the result does not depend on the particular surface choosen. Let the choosen surface be divided into many small loops. If we take the loops small enough, we can assume that each of the small loops enclose an area which is essentially flat. Also we can choose our small loops so that each is very nearly a square. Combining (A.10) with the fact that when you add up the circulation of each individual loop the only remaining contribution comes from the outside edge, we have

$$\int_S \nabla \times \vec{v} \cdot \vec{n} dS = \oint_\Gamma \vec{v} \cdot d\vec{l}. \tag{A.11}$$