6-2015

Partial Differential Equations

Nathaniel James Onnen
Union College - Schenectady, NY

Partial Differential Equations

Nathaniel James Onnen

March 18, 2015

Abstract

This paper will discuss methods for solving many different partial differential equations, as well as real world applications in physics. We are interested in finding solutions to the wave and heat equations in one dimension, the wave equation in two dimensions, as well as a solution to Schrödinger's equation. In order to do this, we will study different methods including Fourier series, Bessel functions, and Hermite polynomials. I will use these methods to derive solutions for the mentioned problems, as well as to produce visualizations for many of them.

Acknowledgements

I would like to thank my advisor, Prof. Jeffrey Jauregui, for all of his help in writing and editing this thesis.

Contents

Chapter 1

Introduction

Mathematical models have been used for centuries to describe how objects move and interact. For this reason, we frequently find many concepts of mathematics tied closely with work in the physical sciences. "Mathematical equations have always provided a context in which to formulate concepts in physics – Maxwell's equations for electrodynamics phenomena, Newton's equations describe mechanical systems, Schrödinger's equation describes aspects of quantum mechanics, and so on." [3] Many of these models are known as **partial differential equations** (PDEs). A PDE is a relation between an unknown function of more than one variable and its partial derivatives.

There are many different methods for solving PDEs. "The classical approach that dominated the nineteenth century was to develop methods for finding explicit solutions." [2] Motivated by the desire to solve problems in physics like the wave and heat equations, different solutions began to emerge. This paper will highlight some of the methods used, as well as their applications in physics.

First, we will begin by developing tools that we use to solve linear partial differential equations. The first tool that we will see for solving PDEs is the Fourier series, developed by the French mathematician Joseph Fourier, "who claimed that any function defined on a finite interval has a Fourier series expansion." [1] Before we can utilize Fourier series, we will first learn about properties of periodic functions, which will be very useful in our study. Then, we can apply Fourier series in the field of physics through the solutions of classic partial differential equations: the wave and heat equations in one dimension.

If we want to study some of these equations in two dimensions, however, we will need even more tools. In this instance, we will study Bessel functions and their properties. Using Bessel functions, we will be able to derive a solution for the two dimensional wave equation. At this point, we will look at other sets of functions, which will be called **orthogonal functions**, that we will use so solve problems in quantum physics.

The paper will conclude with a study of quantum physics, most specifically Schrödinger's equation, which describes the motion of a sub-atomic particle, like an electron. This study will be a culmination of all that was learned in the simpler cases. Like the other problems in physics, a solution will be derived using the superposition of various normal modes.

Chapter 2

Tools for Solving Partial Differential Equations: Fourier Series

One method to solve many linear partial differential equations is through Fourier series. Like Taylor series in calculus, we are attempting to model a function through a series expansion. While the Taylor series focuses on sums of polynomials, the Fourier series is an expansion based on the sums of sines and cosines. It takes the following form for a function f:

$$f(x) = a_0 + \sum_{n=1}^{\infty}(a_n \cos nx + b_n \sin nx) \tag{2.1}$$

The idea is that "any real valued function defined on a closed interval can be represented as a series of trigonometric functions" [2]. As we will see, trigonometric functions like sine and cosine have interesting properties that will allow us to solve classic problems in physics like the wave and heat equation.

2.1 Periodic Functions

When discussing Fourier series, it is important to discuss properties of periodic functions. A function f is **periodic**, or **T-periodic** for a period T, where $T > 0$, if that function satisfies

$$f(x) = f(x+T), \text{ for all x.}$$

For example, the functions sin and cos are 2π-periodic, as

$$\sin x = \sin(x + 2\pi),$$
$$\cos x = \cos(x + 2\pi).$$

We can study some properties of periodic functions that will help us to better understand Fourier Series. When discussing periodic functions, we often refer only to functions that are **piecewise continuous** or **piecewise differentiable**. A function is piecewise continuous on a closed interval $[a, b]$ if it is continuous except possibly at a finite number of points in $[a, b]$, where the function has a simple discontinuity [3]. A function is piecewise differentiable on a closed interval $[a, b]$ if f and f' are are both piecewise continuous on $[a, b]$.

The following theorem shows a property of T-periodic functions that is very useful: the definite integral of a T-periodic function is the same over any interval of length T. This will allow us to change the integrands as needed when evaluation these functions over an interval of length T.

Theorem 2.1.1. [1] *Suppose that f is piecewise continuous and T-periodic. Then for any real number a, we have*

$$\int_0^T f(x)dx = \int_a^{a+T} f(x)dx$$

Proof. The proof of this is fairly simple using the Fundamental Theorem of Calculus. If we assume f is continuous and T-periodic, let $F(a) = \int_a^{a+T} f(x)dx$. Then $F'(a) = f(a+T) - f(a) = 0$, as $f(a+T) = f(a)$ because f is T-periodic. Thus $F(a)$ is constant, so $F(a) = F(0)$, which proves the theorem. □

The most common periodic functions, the trigonometric functions of sine and cosine, have interesting orthogonality properties which will be used frequently in our solutions of different partial differential equations.

Example 2.1.1. *We can also examine the antiderivatives of periodic functions. Suppose that a function f is 2π–periodic, and let a be a real number.*

Define

$$F(x) = \int_a^x f(t)dt, \textit{ for all } x.$$

Show that $F(x)$ *is* 2π*–periodic iff* $\int_0^{2\pi} f(t)dt = 0$.

Proof. Assume $F(x)$ is 2π–periodic. Thus $F(x) = F(x + 2\pi)$. And

$$\begin{aligned} \int_a^x f(t)dt = \int_a^{x+2\pi} f(t)dt &= \int_a^x f(t)dt + \int_x^{x+2\pi} f(t)dt \\ &= \int_a^x f(t)dt + \int_0^{2\pi} f(t)dt \qquad \text{by Theorem 2.1.1} \end{aligned}$$

Therefore, $\int_0^{2\pi} f(t)dt = 0$.

Assume $\int_0^{2\pi} f(t)dt = 0$. Then

$$\begin{aligned} F(x + 2\pi) = \int_a^{x+2\pi} f(t)dt &= \int_a^x f(t)dt + \int_x^{x+2\pi} f(t)dt \\ &= \int_a^x f(t)dt + \int_0^{2\pi} f(t)dt \qquad \text{by Theorem 2.1.1} \\ &= \int_a^x f(t)dt = F(x) \end{aligned}$$

□

The periodic functions that we will be most interested in are the trigonometric functions of sine and cosine. We can see that these are 2π-periodic functions. A property of these functions that we will find useful are their orthogonality properties. For now, we will simply state that two functions f and g are orthogonal on an interval $[a, b]$ if $\int_a^b f(x)g(x)dx = 0$. We will further develop this notion later in the paper. For now, let us consider the following orthogonality properties of sine and cosine.

Proposition 2.1.2. [1]

$$\int_{-\pi}^{\pi} \cos mx \cos nx = 0 \text{ if } m \neq n \text{ for integers } m,\ n. \tag{2.2}$$

$$\int_{-\pi}^{\pi} \cos mx \sin nx = 0 \text{ for all integers } m \text{ and } n \tag{2.3}$$

$$\int_{-\pi}^{\pi} \sin mx \sin nx = 0 \text{ if } m \neq n \text{ for integers } m, \text{ and } n. \tag{2.4}$$

Proof.

$$\begin{aligned}\int_{-\pi}^{\pi} \cos mx \cos nx dx &= \int_{-\pi}^{\pi} \frac{1}{2}[\cos(m+n)x + \cos(m-n)x] \\ &= \frac{1}{2}\left[\frac{1}{m+n}\sin(m+n)x + \frac{1}{m-n}\sin(m-n)x\right]_{-\pi}^{\pi} \\ &= 0,\end{aligned}$$

as if m and n are integers, we know $\sin((m+n)\pi) = 0$ for all m, n such that $m \neq n$. The other equalities can be shown similarly. □

2.2 Fourier Series

As we will see later when we look at applications of partial differential equations in physics, we cannot always explicitly derive the solutions to partial differential equations: for example the one dimensional wave equation which is defined as: $\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial t^2}$. Motivation: How do we solve the wave equation for initial arbitrary amplitude $f(x)$? Idea: We can write f(x) in terms of sines and cosines (i.e. $a_0 + a_1 \cos x + a_2 \cos 2x + ... + b_1 \sin x + b_2 \sin 2x + ...$).

A **Fourier series expansion** of $f(x)$ takes the form:

$$a_0 + \sum_{n=1}^{\infty}(a_n \cos nx + b_n \sin nx) \tag{2.5}$$

We can use the following Euler formulas to determine the coefficients

a_0, a_n, and b_n:

$$a_0 = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x)dx \tag{2.6}$$

$$a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos nx dx \tag{2.7}$$

$$b_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin nx dx \tag{2.8}$$

These can be found by integrating over $[-\pi, \pi]$ on both sides of the equality, and interchanging the operators $\int$ and $\sum$:

$$\int_{-\pi}^{\pi} f(x)dx = \int_{-\pi}^{\pi} a_0 dx + \sum_{n=1}^{\infty} \int_{-\pi}^{\pi} (a_n \cos nx + b_n \sin nx)dx$$

We can see that:

$$\begin{aligned} \int_{-\pi}^{\pi} f(x)dx &= \int_{-\pi}^{\pi} a_0 dx + \sum_{n=1}^{\infty} \left(\frac{a_n}{n} \sin nx + \frac{b_n}{n} \cos nx \right) \Bigg|_{-\pi}^{\pi} \\ &= 2\pi a_0 \end{aligned}$$

Thus,

$$a_0 = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x)dx$$

To solve for a_m, $m > 1$, we will multiply the equality by $\cos mx$, integrate, and interchange $\int$ and $\sum$ once again:

$$\int_{-\pi}^{\pi} f(x) \cos mx dx = \int_{-\pi}^{\pi} a_0 \cos mx dx + \sum_{n=1}^{\infty} \int_{-\pi}^{\pi} (a_n \cos nx \cos mx + b_n \sin nx \cos mx)\, dx$$

Using the orthogonality rules (2.2-2.4), we can see that:

$$\int_{-\pi}^{\pi} f(x) \cos mx dx = a_m \int_{-\pi}^{\pi} \cos^2 mx dx = \pi a_m$$

Thus

$$a_m = \frac{1}{\pi} \int\limits_{-\pi}^{\pi} f(x) \cos mx dx.$$

We can do similar work to show $b_n = \frac{1}{\pi} \int\limits_{-\pi}^{\pi} f(x) \sin mx dx$.

We can denote the $\mathbf{K^{th}}$ **partial sum** of the Fourier Series of f by $S_K(x)$: calculated as:

$$S_K(x) = a_0 + \sum_{n=1}^{K} (a_n \cos nx + b_n \sin nx) \tag{2.9}$$

If we know $f(x)$, we can calculate the error of $S_K(x)$ by:

$$E_K(x) = \int\limits_{0}^{2\pi} (f(x) - S_N(x))^2 dx$$

This tells us how different our partial sum is from the function that we are deriving the Fourier series for.

Example 2.2.1. *Find the Fourier series expansion of $f(x) = |\sin x|$*

Proof. Using the equations for the coefficients of the Fourier series expansion, we see:

$$\begin{aligned}
a_0 &= \frac{1}{2\pi} \int\limits_{-\pi}^{\pi} |\sin x| dx = \frac{4}{2\pi} = \frac{2}{\pi} \\
a_n &= \frac{1}{\pi} \int\limits_{-\pi}^{\pi} |\sin x| \cos nx dx \\
&= \frac{2(1 + \cos n\pi)}{(n^2 - 1)\pi} \\
b_n &= \frac{1}{\pi} \int\limits_{-\pi}^{\pi} |\sin x| \sin nx dx \\
&= 0.
\end{aligned}$$

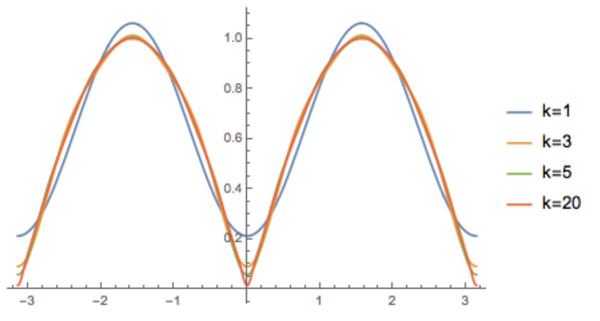

Figure 2.1: Fourier Series representations of $|sinx|$ for various partial sums

Thus the Fourier series expansion of $f(x)$ is:

$$\frac{2}{\pi} + \sum_{n=1}^{\infty} \frac{2(1+\cos n\pi)}{(n^2-1)\pi} \cos nx$$

We can see how as n increases, the Fourier Series approaches $f(x) = |\sin x|$, as we can see in figure (2.1). □

We can use Fourier Series to come up with a fun result: Let $f(x) = x^2$ on $[-\pi, \pi]$. It can be shown that the Fourier Series Expansion for $f(x)$ is:

$$\frac{\pi^2}{3} + 4\sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \cos nx$$

We can use this result to show that $\frac{\pi^2}{6} = 1 + \frac{1}{2^2} + \frac{1}{3^2} + ...$, which is convergent as $\sum_{n=1}^{\infty} \frac{1}{n^2}$ is convergent by the p-test, since $2 > 1$.

$$\begin{aligned}
\pi^2 = f(\pi) &= \frac{\pi^2}{3} + 4\sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \cos n\pi \\
\frac{2\pi^2}{3} &= 4\sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \cos n\pi \\
\frac{\pi^2}{6} &= \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \cos n\pi \\
&= \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} (-1)^n \\
&= \sum_{n=1}^{\infty} \frac{(-1)^{2n}}{n^2} \\
&= \sum_{n=1}^{\infty} \frac{1}{n^2} \\
&= 1 + \frac{1}{2^2} + \frac{1}{3^2} + ...
\end{aligned}$$

So far, all of the functions we have looked at have had period of length 2π, however, not every period has the same length. It is therefore important to represent a Fourier Series of arbitrary period. This will allow us to use Fourier series to tackle a larger variety of problems:

Theorem 2.2.1. [1] *Let f be a 2p-periodic function, where $p > 0$ The Fourier Series expansion is:*

$$f(x) = a_0 + \sum_{n=1}^{\infty} (a_n \cos \frac{n\pi}{p} x + b_n \sin \frac{n\pi}{p} x) \tag{2.10}$$

Where,

$$\begin{aligned}
a_0 &= \frac{1}{2p} \int_{-p}^{p} f(x) dx \\
a_n &= \frac{1}{p} \int_{-p}^{p} f(x) \cos \frac{n\pi}{p} x dx \\
b_n &= \frac{1}{p} \int_{-p}^{p} f(x) \sin \frac{n\pi}{p} x dx
\end{aligned}$$

Recall, a function f is considered to be **even** if $f(-x) = f(x)$ for all x, and f is considered **even** if $f(-x) = -f(x)$ for all x. Also, if a function is even or odd, we can see some interesting results.

Proposition 2.2.2. *Assume f is a 2p-periodic function, with Fourier Series representation (2.10). Then f is even iff* $b_n = 0$ *for all n, and f is odd iff* $a_n = 0$ *for all n.*

Proof. Let $f(x)$ be an even function. Then $f(-x) = f(x)$, for all x. Then,

$$a_0 + \sum_{n=1}^{\infty}\left(a_n \cos\left(\frac{n\pi}{p}x\right) + b_n \sin\left(\frac{n\pi}{p}x\right)\right) = a_0 + \sum_{n=1}^{\infty}\left(a_n \cos\left(-\frac{n\pi}{p}x\right) + b_n \sin\left(-\frac{n\pi}{p}x\right)\right)$$

As cos is even, and sin is odd, we can see

$$\sum_{n=1}^{\infty} b_n \sin\frac{n\pi}{p}x = -\sum_{n=1}^{\infty} b_n \sin\frac{n\pi}{p}x$$

Thus $b_n = 0$, for all n, since the set $\{\sin nx : n = 1, 2, ...\}$ is linearly independent.

Now, assume that $b_n = 0$, for all n, then $f(x) = a_0 + \sum\limits_{n=1}^{\infty} a_n \cos\frac{n\pi}{p}x$. Then, for all x,

$$f(-x) = a_0 + \sum_{n=1}^{\infty} a_n \cos\left(-\frac{n\pi}{p}x\right) = a_0 + \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi}{p}x\right) = f(x)$$

Thus, $f(x)$ is even. It is a similar proof for $f(x)$ odd. □

Example 2.2.2. *Suppose that f is* 2*p-periodic, piecewise-smooth, and continuous, and suppose that* f' *is also piecewise-smooth. If we let* a_n *and* b_n *denote the Fourier coefficients of f and* a'_n *and* b'_n *denote the Fourier coefficients of* f'*. We can show that:*

$$a'_0 = 0,\ a'_n = b_n\frac{n\pi}{p},\ and\ b_n = a_n\frac{n\pi}{p}$$

Proof. Note that we cannot simply differentiate term by term.

$$\begin{aligned} a'_0 &= \frac{1}{2p}\int_{-p}^{p} f'(x)dx \\ &= \frac{1}{2p}\, f(x)|_{-p}^{p}, \qquad \text{by the F.T.C.} \\ &= 0 \end{aligned}$$

$$
\begin{aligned}
a'_n &= \frac{1}{p}\int_{-p}^{p} f'(x)\cos\frac{n\pi}{p}x\,dx \qquad \text{using integration by parts,}\\
&= \frac{1}{p}(f(x)\cos\frac{n\pi}{p}x\big|_{-p}^{p}) + \frac{1}{p}\int_{-p}^{p} f(x)\frac{n\pi}{p}\sin\left(\frac{n\pi}{p}x\right)dx\\
&= \frac{n\pi}{p}(\frac{1}{p}\int_{-p}^{p} f(x)\sin\frac{n\pi}{p}x\,dx)\\
&= \frac{n\pi}{p}b_n
\end{aligned}
$$

It is a similar proof to show that $b_n = -a_n\frac{n\pi}{p}$. □

Sometimes, the function f that we wish to represent with a Fourier series is defined only on a finite interval, like $0 < x < p$. This function f is not periodic, so we must find a way to extend f to a periodic function. This can be done by the **cosine series expansion** and **sine series expansion** of f. If we can extend f to a periodic function, we can represent it using a Fourier series. As cosine is an even function, the cosine series expansion will extend f into an even function. As well, if we apply the sine series expansion, f will be extended to an odd function.

Theorem 2.2.3. *We define the* ***cosine series expansion*** *by*

$$a_0 + \sum_{n=1}^{\infty} a_n \cos\frac{n\pi}{p}x \qquad (0 < x < p)$$

where,

$$a_0 = \frac{1}{p}\int_{0}^{p} f(x)dx; \qquad a_n = \frac{2}{p}\int_{0}^{p} f(x)\cos\frac{n\pi}{p}x\,dx \ (n \geq 1)$$

f also has the ***sine series expansion***

$$\sum_{n=1}^{\infty} b_n \sin\frac{n\pi}{p}x \qquad (0 < x < p)$$

where,

$$b_n = \frac{2}{p}\int_0^p f(x)\sin\frac{n\pi}{p}xdx \qquad (n \geq 1)$$

Example 2.2.3. *We can show the half-range expansions for the function* $f(x) = \pi - x$ *if* $0 \leq x \leq \pi$

Proof. We can use this theorem to find the cosine series expansion:

$$a_0 = \frac{1}{\pi}\int_0^\pi (\pi - x)dx = \frac{1}{\pi}\left(\pi x - \frac{1}{2}x^2\Big|_0^\pi\right) = \frac{1}{\pi}\left(\pi^2 - \frac{1}{2}\pi^2\right) = \frac{1}{2}pi$$

$$\begin{aligned}
a_n &= \frac{2}{\pi}\int_0^\pi (\pi - x)\cos nxdx = \frac{2}{\pi}\int_0^{pi} \pi\cos nx - x\cos nxdx \\
&= 2\sin nx\Big|_0^\pi - \frac{2}{\pi}\int_0^\pi x\cos nxdx \\
&= -\frac{2}{\pi}\left[\frac{x}{n}\sin nx\Big|_0^\pi - \frac{1}{n}\int_0^\pi \sin nxdx\right] \\
&= -\frac{2}{\pi n^2}\left(\cos nx\Big|_0^\pi\right) \\
&= -\frac{2}{\pi n^2}\left[\cos n\pi - 1\right], n = 1, 2, 3, ... \\
&= \frac{4}{\pi(2k+1)^2}
\end{aligned}$$

Thus, the cosine series expansion for $f(x)$ is $\frac{\pi}{2} + \sum_{k=0}^{\infty} \frac{4}{\pi(2k+1)^2}\cos kx$. □

We can see in figure (2.2), how as k increases, the cosine series expansion gets closer to $f(x) = \pi - x$ on the region $0 \leq x \leq \pi$.

2.2.1 Convergence of Fourier Series

When studying Fourier series, it is important to discuss convergence, most importantly uniform convergence. We will see that if the Fourier series representation of some function $u(x)$ converges, and its derivative converges,

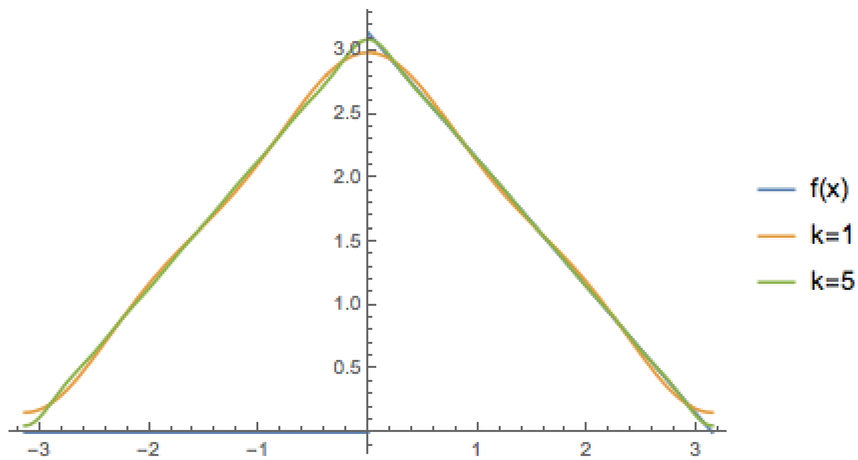

Figure 2.2: Cosine series expansion of $f(x) = \pi - x$ at various partial sums

then $u'(x)$ can be calculated by termwise differentiation. This will aid us greatly in solving partial differential equations.

A sequence of functions, f_n **converges pointwise** on a set $E \subseteq \mathbb{R}$ if $f_n(x)$ converges to $f(x)$ for every $x \in E$. Uniform convergence is a stronger statement. We say that f_n **converges uniformly** on E, if given $\epsilon > 0$, there exists a positive integer N, such that for $n \geq N$, $|f_n(x) - f(x)| < \epsilon$, for all $x \in E$.

Generally, when working with Fourier series, we are not working with a sequence of functions f_n, but instead with a series of functions, usually denoted $\sum_{k=0}^{\infty} u_k(x)$. This series is said to **converge uniformly** on a set E if some sequence of partial sums, $\sum_{k=o}^{n} u_k(x)$ converges to $u(x)$ on E.

There are many tests that can be used to show that a series is convergent, including, but not limited to, the comparison test and the n$^{\text{th}}$ term test, but one of the more useful uniform convergence tests that we will be using is the **Weierstrass M-Test** [1].

The Weierstrass M-Test says given a sequence of functions on a set E, $\{u_k\}_{k=1}^{\infty}$, suppose that there exists a sequence of non-negative real numbers,

$\{M_k\}_{k=0}^{\infty}$ such that the following hold:

$$(1.)\ |u_k(x)| < M_k, \qquad \text{for all } x \in E$$
$$(2.)\ \sum_{k=0}^{\infty} M_k < \infty$$

Then $\sum_{k=0}^{\infty} u_k(x)$ converges uniformly on E.

We can see how the Weierstrass M-Test works in the following example.

Example 2.2.4. *Show that*

$$\sum_{k=1}^{\infty} \left(\frac{\sin kx}{k}\right) e^{-kx} \tag{2.11}$$

converges on all $x \geq 0$.

Take $x \geq \delta$ for some $\delta > 0$. Then

$$\left|(\frac{\sin kx}{k})e^{-kx}\right| \leq \left|\frac{1}{k}e^{-kx}\right| \leq \left|\frac{1}{e^{kx}}\right| \leq \left|\frac{1}{e^{\delta k}}\right|$$

and

$$\sum_{k=1}^{\infty} \frac{1}{e^{\delta k}} < \infty$$

as x is constant as far as k is concerned. Therefore, the above summation converges, as it is a geometric series with $\frac{1}{e^{\delta}} < 1$, using the Weierstrass M-Test. There are also important theorems and corollaries regarding uniform convergence and continuity.

Theorem 2.2.4. [1] *Suppose u_k are continuous functions on a set E If $\sum_{k=0}^{\infty} u_k$ converges uniformly to $u(x)$ on E, then u is continuous on E.*

Corollary 2.2.5. [1] *Given a 2p-periodic function f with Fourier series expansion $a_0 + \sum_{n=1}^{\infty}(a_n \cos\frac{n\pi}{p} + b_n \sin\frac{n\pi}{p})$, then if the Fourier series converges uniformly on f, then f is continuous, and if the Fourier series converges on the interval of length 2p, then the Fourier series converges uniformly, and f is continuous.*

This theorem and corollary allow us to make an interesting statement regarding a Fourier series and termwise differentiation.

Theorem 2.2.6. *Let $E = [a, b]$ and u_k and u'_k are continuous on E, and suppose that $u(x) = \sum_{k=0}^{\infty} u_k(x)$ and $\sum_{k=0}^{\infty} u'_k(x)$ converge uniformly on E. Then $u(x)$ is differentiable on E, and $u'(x) = \sum_{k=0}^{\infty} u'_k(x)$.*

We can show that equation (2.11) from example (2.2.4) is differentiable for all $x > 0$ using this theorem.

Example 2.2.5. *Show that equation 2.11 is differentiable for all $x > 0$. What is its derivative?*

$$
\begin{aligned}
u_n(x) &= \left(\frac{\sin kx}{k}\right) e^{-kx} \\
u'_n(x) &= -ke^{-kx}\left(\frac{\sin kx}{k}\right) + e^{-kx}\left(\frac{k\cos kx}{k}\right) \\
&= e^{-kx}(\cos kx - \sin kx)
\end{aligned}
$$

$$
\begin{aligned}
\left|e^{-kx}(\cos kx - \sin kx)\right| &\leq \left|e^{-kx}(1+1)\right| \\
&= \left|2/e^{kx}\right| \\
&\leq \left|2/e^{\delta k}\right|
\end{aligned}
$$

The sum of this equation converges on $x > 0$, so as $\sum_{k=1}^{\infty} u_k(x)$ and $\sum_{k=1}^{\infty} u'_k(x)$ converge uniformly on $x > 0$, then $u(x) = \sum_{k=1}^{\infty} u_k(x)$ is differentiable on $x \geq 0$ and $u'(x) = \sum_{k=1}^{\infty} u'_k(x)$.

Using the theorems and examples in this section, we will be able to use Fourier series to help us solve partial differential equations.

Chapter 3

Applications in Classical Physics

One of the main applications of partial differential equations come in the area of physics. We can see these applications in the one dimensional wave equation, which can model the motion of a 1-D wave over time, and the one dimensional heat equation, which models the temperature of a thin rod over time. These equations can be seen below:

$$\text{One dimensional wave equation: } \frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \tag{3.1}$$

$$\text{One dimensional heat equation: } \frac{\partial u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \tag{3.2}$$

where c is a constant, and $c > 0$.

3.1 The Wave Equation

We can use partial differential equations to model a vibrating string. In this instance, we are considering "a uniform string undergoing transversal motion whose amplitude is denoted by $u(x, t)$, where x is the spatial coordinate, and t denotes time" [2]. However, in order to do this, some assumptions must be made about the string [1]:

1. The string has a constant mass density ρ (**homogeneous string**)
2. The string is perfectly elastic and offers no resistance to bending (i.e. we need to only consider an external force of gravity and the internal force of tension)

3. The motion of the string is transverse only (this implies the horizontal component of the tension is the same at all points). The transverse vibrations of the string are small and take place in a plane containing the x-axis, the xu-plane. Also, the slope at any point go the string, $\partial u/\partial x$, is small.

We have already seen the equation for a one dimensional wave in equation (3.1). We can find the solution to u with given **boundary conditions** for a string of length L:

$$u(0,t) = 0 \text{ and } u(L,t) = 0 \text{ for all } t > 0,$$

meaning that the ends of the string are fixed at 0. The equation also has the following **initial conditions**:

$$u(x,0) = f(x) \text{ and } \frac{\partial u}{\partial t}(x,0) = g(x) \text{ for } 0 < x < L$$

This gives us an initial position function for time 0, $f(x)$, and an initial velocity function at time 0, $g(x)$.

We will find a solution to the wave equation by using separation of variables. This method of finding a solution is called an **anzatz**, which is an assumption of the form of an unknown function, in order to find a solution to the given problem. We assume that the solution of the one dimensional wave equation takes the form:

$$u(x,t) = X(x)T(t)$$

For our solution, $X(x)$ is a function of x alone, and $T(t)$ is a function of t alone. Thus:

$$u_{xx} = X''(x)T(t) \text{ and } u_{tt} = X(x)T''(t)$$

We can plug these equations into Equation 3.1 to yield:

$$c^2[X''(x)T(t)] = X(x)T''(t)$$
$$\frac{X''(x)}{X(x)} = \frac{T''(t)}{c^2T(t)}$$

These equations are separated, as the function on the left is a function of x alone, and the function on the right is a function of t alone. As x and t

are independent of each other, the only way that these two equations can be equal are if they both equal some constant k :

$$X'' = kX \text{ and } T'' = kc^2 T$$

We can rule out the cases where $k > 0$ and $k = 0$, as $k > 0$ yields a general solution of the form $X(x) = c_1 \cosh \mu x + c_2 \sinh \mu x$ for $\mu > 0$. Using the boundary conditions, we can see that the only c_1, c_2, that satisfy the boundary conditions is $c_1 = c_2 = 0$. If $k = 0$, we get a general solution of the form $X(x) = c_1 x + c_2$. Using the boundary conditions, we see again we must take $c_1 = c_2 = 0$. Thus we solve these ODEs for $k < 0$. If we assume that $k = -\mu^2 < 0$, $\mu > 0$, then we can see that:

$$X'' + \mu^2 X = 0,\ X(0) = 0 \text{ and } X(L) = 0$$

We can see that a general solution to this equation is:

$$X = c_1 \cos \mu x + c_2 \sin \mu x.$$

Using the boundary condition of $X(0) = 0$, we can see that $c_1 = 0$, so let's say that $c_2 \neq 0$, in order to avoid a trivial solution, thus:

$$\sin \mu L = 0$$

due to the boundary condition $X(L) = 0$ As the sine function is 0 at integer multiples of π, we can see that

$$\mu = \mu_n = \frac{n\pi}{L}, n = \pm 1, \pm 2, ...$$

and so,

$$X = X_n = \sin\left(\frac{n\pi}{L} x\right), n = 1, 2, ...$$

We can also use $k = -\mu^2 = -(\frac{n\pi}{L})^2$ to get the following equation:

$$T'' + (c\frac{n\pi}{L})^2 T = 0$$

We can substitute in $\lambda_n = c\frac{n\pi}{L}$. Then,

$$T_n = b_n \cos \lambda_n t + b_n^* \sin \lambda_n t$$

Where b_n, b_n^* are unknown coefficients.

Substituting this equation and the equation for X_n, we can see:

$$u_n(x,t) = \sin\left(\frac{n\pi}{L}x\right)(b_n \cos \lambda_n t + b_n^* \sin \lambda_n t), \qquad n = 1, 2, ...$$

are the **normal modes** of the wave equation.

We can guess that the solution, $u(x,t)$ will be some infinite sum of the u_n, and submit

$$u(x,t) = \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{L}x\right)(b_n \cos \lambda_n t + b_n^* \sin \lambda_n t)$$

as a solution of the boundary value problem. In order to completely derive a solution for the wave equation, we need to determine values for b_n and b_n^*

We can use our initial conditions to help solve for these coefficients. Plugging in $u(x,0)$, we get:

$$u(x,0) = f(x) = \sum_{n=1}^{\infty} b_n \sin \frac{n\pi}{L},\ 0 < x < L$$

We can recall that this is the same as the sine series expansion for a function $f(x)$(Chapter 2, Section2). Thus we we can solve for b_n as follows:

$$b_n = \frac{2}{L} \int_0^L f(x) \sin \frac{n\pi}{L} dx$$

We use the second initial condition to solve for b_n^*:

$$\frac{\partial u}{\partial t}(x,0) = g(x) = \sum_{n=1}^{\infty} b_n^* \lambda_n \sin \frac{n\pi}{L} x$$

This is the sine series expansion for $g(x)$, so we get:

$$b_n^* \lambda_n = \frac{2}{L} \int_0^L g(x) \sin \frac{n\pi}{L} x dx$$

$$b_n^* (c\frac{n\pi}{L}) = \frac{2}{L} \int_0^L g(x) \sin \frac{n\pi}{L} x dx$$

$$b_n^* = \frac{2}{cn\pi} \int_0^L g(x) \sin \frac{n\pi}{L} x dx$$

We can use these equations to solve for the the solution of the wave equation with various initial conditions:

Example 3.1.1. *Solve the boundary value problem for the wave equation with the following conditions:*

$$f(x) = \sin \pi x + 3\sin 2\pi x - \sin 5\pi x$$
$$g(x) = 0,\ c = 1$$

Proof. As $g(x) = 0$, $b_n^* = 0$.

We can use the above equation to solve for b_n:

$$b_n = 2\int_0^1 [\sin \pi x + 3\sin 2\pi x - \sin 5\pi x] \sin n\pi x dx$$
$$= 2\int_0^1 \sin \pi x \sin n\pi x dx + 6\int_0^1 \sin 2\pi x \sin n\pi x dx - 2\int_0^1 \sin 5\pi x \sin n\pi x dx$$

We can see, using the orthogonality properties of sin, that $b_n = 1, 3, -1$ when $n = 1, 2, 5$ respectively, and 0 otherwise. So,

$$u(x,t) = \sum_{n=1}^{\infty} \sin n\pi x[b_n \cos n\pi t]$$

Thus:

$$u(x,t) = \sin \pi x \cos \pi t + 3\sin 3\pi x \cos 3\pi t - \sin 5\pi x \cos 5\pi t$$

We can see how the string moves in figure (3.1). □

Let's also see an example when $g(x) \neq 0$:

Example 3.1.2. *Solve the boundary value problem for the wave equation with the following conditions:*

$$f(x) = \begin{cases} 0, \ \mathit{if}\ 0 \le x \le \frac{1}{3} \\ \frac{1}{30}(x - \frac{1}{3}), \ \mathit{if}\ \frac{1}{3} \le x \le \frac{2}{3} \\ \frac{1}{30}(1-x) \ \mathit{if}\ \frac{2}{3} \le x \le 1 \end{cases} \qquad g(x) = 2, c = \frac{1}{\pi}$$

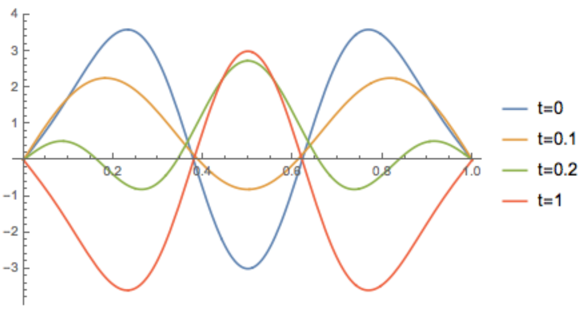

Figure 3.1: Graph of the solution $u(x,t)$

Proof. Let us first solve for b_n

$$b_n = 2\int_0^{\frac{1}{3}} 0 \sin n\pi x dx + \frac{1}{15}\int_{\frac{1}{3}}^{\frac{2}{3}} (x - \frac{1}{3}) \sin n\pi x dx + \frac{1}{15}\int_{\frac{2}{3}}^{1} (1 - x) \sin n\pi x dx$$

We can use integration by parts to show that

$$b_n = \frac{1}{15}\left[-\frac{2\cos\frac{2n\pi}{3}}{3n\pi} + \frac{2\sin\frac{2n\pi}{3}}{n\pi} - \frac{\sin\frac{n\pi}{3}}{n\pi} \right]$$

Now, let's solve for b_n^*:

$$\begin{aligned} b_n^* &= \frac{2}{n}\int_0^1 2\sin n\pi x dx \\ &= -\frac{4}{n^2}\cos n\pi x\Big|_0^1 \\ &= -\frac{4}{n^2}(\cos n\pi - 1) \\ &= -\frac{8}{(2n+1)^2} \end{aligned}$$

We can also see that $\lambda_n = n$, thus:

$$u(x,t) = \sum_{n=1}^{\infty} \sin n\pi x \left(\frac{1}{15}\left[-\frac{2\cos\frac{2n\pi}{3}}{3n\pi} + \frac{2\sin\frac{2n\pi}{3} - \sin\frac{n\pi}{3}}{n\pi} \right] \cos nt - \frac{8}{(2n+1)^2}\sin nt \right)$$

□

3.2 The Heat Equation

We can also use partial differential equations to model the temperature of a point x of a bar at a time t. Recall, that the **one dimensional heat equation** is represented by the equation:

$$\frac{\partial u}{\partial t} = c^2 \frac{\partial^2 u}{\partial x^2}, \qquad 0 < x < L, \qquad t > 0$$

Like the one dimensional wave equation, the heat equation has boundary conditions:

$$u(0,t) = 0 \text{ and } u(L,t) = 0 \text{ for all } t > 0$$

which means that the ends of the rods have a temperature of 0 regardless of time. The heat equation also has the initial condition:

$$u(x,0) = f(x) \text{ for } 0 < x < L$$

which is the initial temperature distribution of the bar. Like with the wave equation, we will assume the solution u takes the form

$$u(x,t) = X(x)T(t)$$

We plug this solution into the heat equation to get:

$$\frac{T'}{c^2 T} = \frac{X''}{X}$$

Thus, we can see that

$$\frac{T'}{c^2 T} = k \text{ and } \frac{X''}{X} = k$$

We use these to generate the following two ordinary differential equations:

$$T'' - kc^2 T = 0$$
$$\text{and}$$
$$X'' - kX = 0$$

Using the boundary conditions we see that:

$$X(0)T(t) = 0$$
$$\text{and}$$
$$X(L)T(t) = 0 \text{ for all } t > 0$$

In order to avoid trivial solutions, let $X(0) = 0$, and $X(L) = 0$, otherwise $T(t) = 0$, for all t. We can use these to obtain a boundary value problem for $X(x)$:

$$X'' - kX = 0, X(0) = 0, \text{ and } X(L) = 0$$

We see that this is the same equation for $X(x)$ that we saw for with the wave equation, so we know $k = -\mu^2$, where $\mu = \mu_n = \frac{n\pi}{L}$, for $n = 1, 2, ...$ Thus:

$$X = X_n = \sin \frac{n\pi}{L} x, n = 1, 2, ...$$

We can use our value of k and substitute it into the differential equation for T:

$$T' + \left(c\frac{n\pi}{L}\right)^2 T = 0 \tag{3.3}$$

It can be shown that the general solution for T_n is:

$$T_n(t) = b_n e^{-\lambda_n^2 t}, n = 1, 2, ...$$

As

$$T_n'(t) = -\lambda_n^2 b_n e^{-\lambda_n^2 t}$$

So,

$$T' + \lambda_n^2 T = -\lambda_n^2 b_n e^{-\lambda_n^2 t} + \lambda_n^2 b_n e^{-\lambda_n^2 t} = 0$$

where $\lambda_n = c\frac{n\pi}{L}$ as with the wave equation. Therefore, the product solution for the one dimensional wave equation with these boundary conditions is:

$$u_n(x, t) = b_n e^{-\lambda_n^2 t} \sin \frac{n\pi}{L} x, \qquad n = 1, 2, ...$$

and

$$u(x, t) = \sum_{n=1}^{\infty} b_n e^{-\lambda_n^2 t} \sin \frac{n\pi}{L} x$$

Again, if we plug in $t = 0$ for our initial condition, we see that:

$$f(x) = u(x, 0) = \sum_{n=1}^{\infty} b_n \sin \frac{n\pi}{L} x$$

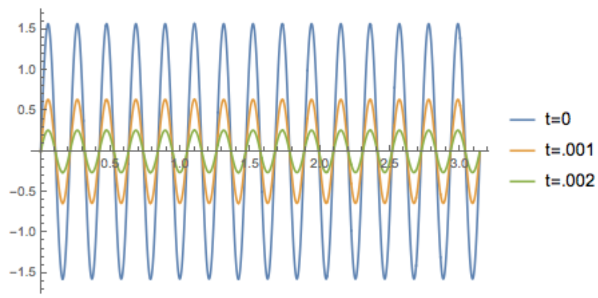

Figure 3.2: Graph of the solution to the heat equation, $u(x, t)$

We also recognize this as the half range sine expansion of f, so we can write

$$b_n = \frac{2}{L} \int_0^L f(x) \sin \frac{n\pi}{L} x dx, n = 1, 2, ...$$

We can see how this solution is used with an example:

Example 3.2.1. *Given a rod of length π, $c = 1$, and $f(x) = \sin 30x$, solve the boundary value heat problem.*

Proof. Let us first solve for b_n:

$$\begin{aligned} b_n &= \frac{2}{\pi} \int_0^\pi \sin 30x \sin nx dx \\ &= 0 \text{ for } n \neq 0, \frac{\pi}{2} \text{ otherwise} \end{aligned}$$

As $\lambda_n = n$, for $n = 1, 2, ...$, we can see that our solution is:

$$u(x, t) = \frac{\pi}{2} e^{-30^2 t} \sin 30x$$

□

We can see how the heat diffuses throughout this rod at different points in time in figure (3.2)

Our solution becomes a little different, however, if we consider a problem where the endpoints are not both at zero. Let us consider the following initial condition for a rod of length 1:

$$f(x) = \begin{cases} 50 & \text{for } 0 \le x \le 1/2 \\ 0 & \text{for } 1/2 \le x \le 1 \end{cases}$$

As t approaches ∞, the temperature distribution is a function of x alone, called the **steady state solution** (or time-independent solution). In the previous example, as both endpoints were 0, the steady state solution was 0. In general, since the steady-state solution is independent of t, then $\partial u/\partial t = 0$. If we plug this into the one dimensional heat equation, we see that the steady-state distribution satisfies $\frac{\partial^2 u}{\partial x^2} = 0$, as the steady-state solution u is a function of x only. Thus, we can find a general solution of this differential equation, $Ax + B = 0$, where A and B are constants that we can determine with the boundary conditions. When finding a solution to the wave equation with nonzero boundary conditions be first find the steady state solution corresponding to the boundary conditions, calculated by:

$$u_1(x) = \frac{T_2 - T_1}{L} x + T_1$$

If we subtract u_1 from the initial temperature distribution, we get the resulting heat boundary value problem

$$\begin{aligned} &\frac{\partial u}{\partial t} = c^2 \frac{\partial^2 u}{\partial x^2}, \qquad 0 < x < L, \qquad t > 0, \\ &u(0,t) = 0 \text{ and } u(L,t) = 0, \qquad t > 0, \\ &u(x,0) = f(x) - u_1(x), \qquad 0 < x < L \end{aligned}$$

If we let $u_2(x,t)$ be the solution to this problem, then by our solution in the case where both ends were 0:

$$u_2(x,t) = \sum_{n=1}^{\infty} b_n e^{-\lambda_n^2 t} \sin\left(\frac{n\pi}{L} x\right)$$

where $\lambda_n = \frac{cn\pi}{L}$, and

$$b_n = \frac{2}{L} \int_0^L \left(f(x) - \left(\frac{T_2 - T_1}{L} x + T_1 \right) \right) \sin\left(\frac{n\pi}{L} x\right) dx.$$

Our solution, $u(x,t)$ is obtained by adding $u_2(x,t)$ to the steady-state solution:

$$u(x,t) = u_1(x,t) = u_2(x,t)$$

Example 3.2.2. *Given a rod of length 1, $c = 1$ and*

$$f(x) = \begin{cases} 50 & \text{for } 0 \leq x \leq 1/2 \\ 0 & \text{for } 1/2 \leq x \leq 1 \end{cases},$$

solve the boundary value heat problem.

Proof. Let us first find the steady-state solution, u_1:

$$u_1(x) = \frac{0-50}{1}x + 50 = -50x + 50$$

We can see that $\lambda_n = n\pi$, so we can now begin to solve for b_n:

$$\begin{aligned}
b_n &= 2\int_0^1 (f(x) - (-50x+50)) \sin n\pi x dx \\
&= 2\left[\int_0^{1/2} (50 - (-50x+50)) \sin n\pi x dx + \int_{1/2}^1 (0 - (-50x+50)) \sin n\pi x dx\right] \\
&= 2\left[\int_0^{1/2} 50x \sin n\pi x dx + \int_{1/2}^1 (50x - 50) \sin n\pi x dx\right] \\
&= 100\left[\int_0^1 x sin n\pi x dx - \int_{1/2}^1 \sin n\pi x dx\right] \\
&= 100\left[-\frac{1}{n\pi} x \cos n\pi x\Big|_0^1 + \frac{1}{n\pi}\int_0^1 \cos n\pi x dx + \frac{1}{n\pi}\cos n\pi x\Big|_{1/2}^1\right] \qquad \text{using IBP} \\
&= 100\left[-\frac{1}{n\pi}\cos n\pi + \frac{1}{n^2\pi^2}\sin n\pi x\Big|_0^1 + \frac{1}{n\pi}\cos n\pi - \frac{1}{n\pi}\cos\frac{n\pi}{2}\right] \\
&= 100\left[-\frac{1}{n\pi}\cos\frac{n\pi}{2}\right].
\end{aligned}$$

Thus,

$$u_2(x,t) = \sum_{n=1}^{\infty} 100\left[-\frac{1}{n\pi}\cos\frac{n\pi}{2}\right] e^{-n^2\pi^2 t} \sin n\pi x.$$

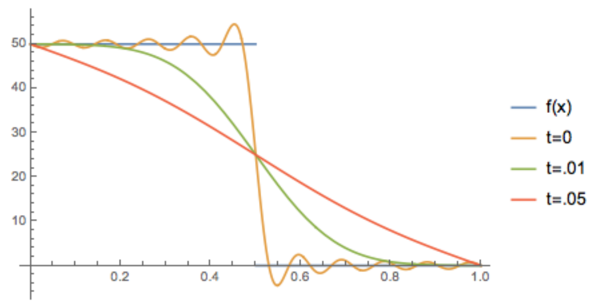

Figure 3.3: Graph of the heat equation with non-zero endpoints at different time steps, with initial condition $f(x)$

When n is odd, we see that b_n is zero, therefore,

$$u_2(x,t) = 100\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{(2k)\pi}e^{-(2k)^2\pi^2 t}\sin 2k\pi x.$$

So,

$$u(x,t) = -50x + 50 + 100\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{(2k)\pi}e^{-(2k)^2\pi^2 t}\sin 2k\pi x. \tag{3.4}$$

□

We can see a visualization of this solution in figure (3.3). Notice how the graph approaches the steady-state solution as the time increases.

Chapter 4

Bessel Functions

As partial differential equations get more complex, we need different methods. As we will see, when studying the 2D wave equation with circular symmetry, the methods we have looked at to this point are not adequate for finding and defining a solution.

We can look at **Bessel's equation of order p**:

$$x^2y'' + xy' + (x^2 - p^2)y = 0 \tag{4.1}$$

Where $p \geq 0$ is a real constant. To find a solution to this ODE, let us use another Ansatz: this time we will assume that the solution takes the form of a power series:

$$y = \sum_{n=0}^{\infty} a_n x^{n+r} \qquad \text{with constant } r$$

Then

$$y' = \sum_{n=0}^{\infty} (n+r) a_n x^{n+r-1}$$

and

$$y'' = \sum_{n=0}^{\infty} (n+r-1)(n+r) a_n x^{n+r-2}$$

Plugging these into equation (4.1), we get:

$$0 = x^2 \sum_{n=0}^{\infty} (n+r-1)(n+r)a_n x^{n+r-2} + x \sum_{n=0}^{\infty} (n+r)a_n x^{n+r-1} + (x^2 - p^2) \sum_{n=0}^{\infty} a_n x^{n+r}$$

$$0 = \sum_{n=0}^{\infty} (n+r-1)(n+r)a_n x^{n+r} + \sum_{n=0}^{\infty} (n+r)a_n x^{n+r} + \sum_{n=2}^{\infty} a_{n-2} x^{n+r} + p^2 \sum_{n=0}^{\infty} a_n x^{n+r}$$

We can write out the $n = 0$ and $n = 1$ terms of the first, second, and fourth summations so that the everything else can be written as a summation from 0 to ∞:

$$\begin{aligned} 0 = a_0 \left(r(r-1) + r - p^2\right) x^r + a_1 \left(r(r+1) + (r+1) - p^2\right) x^{r+1} \\ + \sum_{n=2}^{\infty} \left[\left((n+r)(n+r-1) + (n+r) - p^2\right) a_n + a_{n-2}\right] x^{n+r} \end{aligned}$$

If we simplify the x^r and x^{r+1} terms, we get

$$0 = a_0(r^2 - p^2)$$

$$0 = a_1((r+1)^2 - p^2)$$

Using the summation, we also get the following equation for a_n:

$$a_n = -\frac{a_{n-2}}{(n+r)^2 - p^2}, \text{ for } n \geq 2$$

If we assume $a_0 = 1$, then we get the result $r = \pm p$. If we also assume $r = +p$, then we see that $a_1 = 0$. By the way we define a_n, any odd n would make $a_n = 0$. If n is even, we can see:

$$a_n = -\frac{a_{n-2}}{(n+p)^2 - p^2} = -\frac{a_{n-2}}{n(n+2p)}$$

. We can see that in general:

$$a_{2k} = \frac{(-1)^k}{2^{2k} k!(p+1)(p+2)...(p+k)}, \text{ for } k \geq 1.$$

Therefore, we can define the solution to the Bessel Equation of order p as:

$$J_p(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{2^{2k} k!(p+1)(p+2)...(p+k)} x^{2k+p} \tag{4.2}$$

In figure (4.1) we can see the plots of $J_0(x)$ and $J_1(x)$. We can see, and will show later, that $J_0(x)$ is a lot like $\cos x$ and $J_1(x)$ is a lot like $\sin x$. However, we must first show that $J_p(x)$ is actually a solution to a Bessel equation of order p:

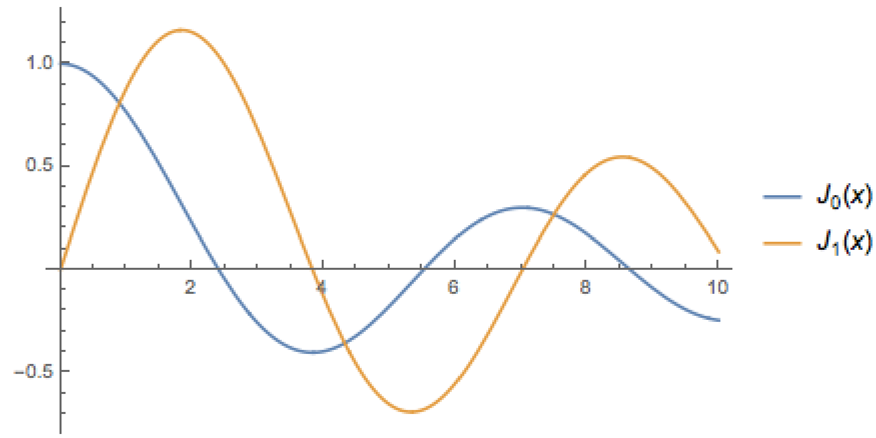

Figure 4.1: Graphs plotting the partial sums of $J_0(x)$ and $J_1(x)$ from $k = 0$ to $k = 50$

Proof. We will first show that $J_p(x)$ converges on all values of x. This will be done using the Ratio Test:

$$\begin{aligned} L &= \lim_{n\to\infty} \left| \frac{\frac{(-1)^{n+1}}{2^{2(n+1)}(n+1)!(p+1)...(p+n)(p+n+1)}}{\frac{(-1)^n}{2^{2n}(n!)(p+1)...(p+n)}} \right| \\ &= \lim_{n\to\infty} \left| \frac{2^{2n}(n!)(p+1)...(p+n)(1)^{n+1}}{2^{2(n+1)}(n+1)!(p+1)...(p+n)(p+n+1)(-1)^n} \right| \\ &= \lim_{n\to\infty} \left| \frac{-1}{4(n+1)(p+n+1)} \right| = 0. \end{aligned}$$

Thus $J_p(x)$ converges on all values of x.

We can see that the above ratio is independent of x, provided that x is limited to a fixed interval $[a, b]$. This would make the rate of convergence independent on x, we can see that $J_p(x)$ is uniformly convergent on the interval $[a, b]$. Thus it is continuous on the whole interval, and therefore on $[0, \infty)$.

As $J_p(x)$ is uniformly convergent, if we can show that the termwise differentiated series is uniformly convergent, then $J_p'(x)$ is the termwise differentiated series. Again, we will use the ratio test to see that this is the case:

$$\begin{aligned}
L &= \lim_{n\to\infty}\left|\frac{\frac{(-1)^{n+1}(2(n+1)+p)}{2^{2(n+1)}(n+1)!(p+1)...(p+n)(p+n+1)}}{\frac{(-1)^n(2n+p)}{2^{2n}(n!)(p+1)...(p+n)}}\right| \\
&= \lim_{n\to\infty}\left|\frac{2^{2n}(n!)(p+1)...(p+n)(1)^{n+1}(2(n+1)+p)}{2^{2(n+1)}(n+1)!(p+1)...(p+n)(p+n+1)(-1)^n(2n+p)}\right| \\
&= \lim_{n\to\infty}\left|\frac{(-1)(2n+p+2)}{4(n+1)(p+n+1)(2n+p)}\right| = 0.
\end{aligned}$$

Thus, $J_p'(x)$ is the termwise differentiated series of $J_p(x)$, by Theorem 2.2.6. A similar argument is made to show that $J_p''(x)$ is the termwise differentiated series of $J_p'(x)$. Therefore, we can see that $J_p(x)$ is a solution to Bessel's Equation, using termwise differentiation. □

4.1 Properties of Bessel Functions

We can see some interesting relationships between Bessel functions, especially those for values of p that differ by whole numbers:

Proposition 4.1.1. *For any $p \geq 0$,*

$$\frac{d}{dx}(x^p J_p(x)) = x^p J_{p-1}(x),$$

and

$$\frac{d}{dx}(x^{-p} J_p(x)) = -x^{-p} J_{p+1}(x)$$

Proof.

$$\begin{aligned}
\frac{d}{dx}\left(x^p J_p(x)\right) &= \frac{d}{dx}\left(\sum_{k=0}^{\infty}\frac{(-1)^k}{2^{2k}(k!)(p+1)...(p+k)}x^{2(k+p)}\right) \\
&= \sum_{k=0}^{\infty}\frac{(-1)^k}{2^{2k}(k!)(p+1)...(p+k)}(2k+2p)x^{2k+2p-1} \\
&= x^p\sum_{k=0}^{\infty}\frac{(-1)^k 2(p+k)}{2^{2k}(k!)(p+1)...(p+k)}x^{2k+(p-1)} \\
&= x^p\sum_{k=0}^{\infty}\frac{(-1)^k}{2^{2k-1}(k!)(p+1)...((p-1)+k)}x^{2k+(p-1)} \\
&= x^p J_{p-1}(x)
\end{aligned}$$

The proof to show $\frac{d}{dx}(x^{-p}J_p(x)) = -x^{-p}J_{p+1}(x)$ is similar. □

We can use this proposition to show the following about $J_0(x)$ and $J_1(x)$:

Corollary 4.1.2. $J_0(x) = -J_1'(x)$

Proof.

$$\begin{aligned}\frac{d}{dx}(J_0(x)) &= \frac{d}{dx}\left(x^0 J_0(x)\right)\\ &= -x^0 J_{0+1}(x)\text{(by the proposition)}\\ &= -J_1(x)\end{aligned}$$

□

So we can see in figure (4.1), that $J_1(x)$ is the negative derivative of $J_0(x)$.

Proposition 4.1.3. *For* $p \geq 1$,

$$J_{p-1}(x) + J_{p+1}(x) = \frac{2p}{x}J_p(x)$$

Proof.

$$\begin{aligned}J_{p-1}(x) + J_{p+1}(x) &= \frac{\frac{d}{dx}(x^p J_p(x))}{x^p} + \frac{\frac{d}{dx}(x^{-p}J_p(x))}{-x^{-p}}\\ &= \frac{x^p J_p'(x) + px^{p-1}J_p(x)}{x^p} + \frac{x^p J_p'(x) - px^{-p-1}J_p(x)}{-x^{-p}}\\ &= J_p'(x) + px^{-1}J_p(x) - J_p'(x) + px^{-1}J_p(x)\\ &= 2px^{-1}J_p(x)\\ &= \frac{2p}{x}J_p(x)\end{aligned}$$

□

4.1.1 Zeroes of the Bessel Functions

We are interested in the zeroes of the Bessel functions like we are in the zeros of other functions, such as sine and cosine. As we can see in figure (4.1), the zeroes form an infinite sequence increasing to infinity. These zeroes of the Bessel function are analogous to the solutions that we saw with the one dimensional wave equation with $\sin\frac{n\pi}{L}x$. We will use these solutions in a similar way when using Bessel functions to solve partial differential equations, which we will see in the next section.

4.1.2 Orthogonality of Bessel Functions

One of the main reasons that we are interested in Bessel functions as a solution to partial differential equations is because like sin and cos, they have orthogonality properties that we can utilize in our solutions.

Proposition 4.1.4. *If $j \neq k$ are both positive integers, then*

$$\int_0^1 J_n(\alpha_{n,j}x)J_n(\alpha_{n,k}x)x dx = 0,$$

where $\alpha_{n,j}$ is the j^{th} zero of $J_n(x)$.

Proof. Fix $a, b > 0$. First, we will show that $J_n(ax)$ and $J_n(bx)$ are solutions to the following ODEs, respectively:

$$x^2y'' + xy' + (a^2x^2 - n^2)y = 0 \tag{4.3}$$
$$x^2y'' + xy' + (b^2x^2 - n^2)y = 0$$

First, note that $J_n(u)$ is a solution to the following Bessel's equation of order n:

$$u^2\frac{d^2}{du^2}(J_n(u)) + u\frac{d}{du}(J_n(u)) + (u^2 - n^2)J_n(u) = 0$$

Replacing $u = ax$, we see:

$$a^2x^2\frac{d^2}{dx^2}(J_n(ax)) + ax\frac{d}{dx}(J_n(ax)) + (a^2x^2 - n^2)J_n(ax) = 0$$

Where $\frac{d}{dx} = \frac{du}{dx}\frac{d}{du}$. Then,

$$a^2x^2\left(\frac{1}{a^2}\right)J_n''(ax) + ax\left(\frac{1}{a}\right)J_n'(ax) + (a^2x^2 - n^2)J_n(ax) = 0$$

Thus,

$$x^2J_n''(ax) + xJ_n(ax) + (a^2x^2 - n^2)J_n(ax) = 0$$

The proof for $J_n(bx)$ is similar. If we divide equation (4.3) by x, we get:

$$xJ_n''(ax) + J_n'(ax) + \left(a^2x - \frac{n^2}{x}\right)J_n(ax) = 0$$
$$\frac{d}{dx}\left(xJ_n'(ax)\right) = -\left(a^2x - \frac{n^2}{x}\right)J_n(ax)$$

Multiplying both sides of this equation by $J_n(bx)$ yields:

$$\frac{d}{dx}\left(xJ_n'(ax)\right)J_n(bx) = -\left(a^2x - \frac{n^2}{x}\right)J_n(ax)J_n(bx)$$

We can take the integral of both sides as follows:

$$\int_0^1 \frac{d}{dx}\left(xJ_n'(ax)\right)J_n(bx)dx = -\int_0^1 \left(a^2x - \frac{n^2}{x}\right)J_n(ax)J_n(bx)dx$$

$$xJ_n'(ax)J_n(bx)\Big|_0^1 - \int_0^1 xJ_n'(ax)\frac{d}{dx}\left(J_n(bx)\right)dx = -\int_0^1 \left(a^2x - \frac{n^2}{x}\right)J_n(ax)J_n(bx)dx$$

$$J_n'(a)J_n(b) - \int_0^1 xJ_n'(ax)\frac{d}{dx}\left(J_n(bx)\right)dx = -\int_0^1 \left(a^2x - \frac{n^2}{x}\right)J_n(ax)J_n(bx)dx$$

We will call this equation $(*_a)$. Similarly, we will represent $(*_b)$ by:

$$J_n'(b)J_n(a) - \int_0^1 xJ_n'(bx)\frac{d}{dx}\left(J_n(ax)\right)dx = -\int_0^1 \left(b^2x - \frac{n^2}{x}\right)J_n(bx)J_n(ax)dx$$

If we suppose that a, and b are distinct zeroes of $J_n(x)$, then $(*_a - *_b)$ becomes:

$$\int_0^1 x\left[J_n'(ax)\frac{d}{dx}\left(J_n(bx)\right) - J_n'(bx)\frac{d}{dx}\left(J_n(ax)\right)\right]dx$$

$$= (a^2 - b^2)\int_0^1 J_n(ax)J_n(bx)xdx$$

□

4.2 Applications of Bessel Functions: Symmetric Vibrations of a Circular Membrane

The two dimensional wave equation is written as

$$\frac{\partial^2 u}{\partial t^2} = c^2\left(\frac{partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right).$$

In this case, and in equations with higher dimensions, we refer to $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$ as the **Laplacian** of u, denoted δu.We can convert the Laplacian into polar coordinates, and can see that the **two dimensional wave equation** in polar coordinates is written as:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} \right) \tag{4.4}$$

We are studying the case of symmetric vibrations, $\frac{\partial u}{\partial \theta} = 0$, so equation (4.4) becomes

$$\frac{\partial^2 u}{\partial t^2} = c^2 \left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} \right) \tag{4.5}$$

We define the membrane as clamped at the edges, so we have a **boundary condition**:

$$u(a,t) = 0, \qquad t \geq 0,$$

Where $0 < r < a$ and $t > 0$. This means that the edge of the membrane is held at zero for all points in time.

We also have the following **initial conditions**:

$$u(r,0) = f(r), \frac{\partial u}{\partial t}(r,0) = g(r), 0 < r < a$$

Where $f(r)$ is the initial position of the membrane, and $g(r)$ is the initial velocity of the membrane. Similarly to the one dimensional wave equation and one dimensional heat equation, a solution can be found using the separation of variable method. If we assume that the solution is of the form:

$$u(r,t) = R(r)T(t)$$

Then we can find the solutions of R and T by first plugging them into equation (4.5) and separating the variables. We see that:

$$\frac{T'}{c^2 T} = \frac{1}{R}\left(R'' + \frac{1}{r}R' \right) = -\lambda^2$$

for some constant λ. The sign of the constant is set to be negative because we expect T to have a periodic solution. So,

$$\begin{aligned} &rR'' + R' + \lambda^2 r R = 0, \qquad R(a) = 0 \\ &T'' + c^2\lambda^2 T = 0 \end{aligned} \tag{4.6}$$

We can see that equation (4.6) is a Bessel's equation of order zero in parametric form. However, the equation is second order and homogeneous, so we need two different linearly independent solutions o write a solution. Therefore we will need to use Bessel functions of order 0 of the first and second kind, denoted: $J_0(\lambda r)$ and $Y_0(\lambda r)$ respectively. Then,

$$R(r) = c_1 J_0(\lambda r) + c_2 Y_0(\lambda r)$$

Since this equation is rooted in the physical world, we expect the solutions to the wave equation to be bounded at all r. Y_0 is unbounded as r approaches 0, so we must choose $c_2 = 1$. If we want to avoid a trivial solution, we select $c_1 = 1$, so,

$$R(r) = J_0(\lambda r)$$

Applying the condition $R(a) = 0$, we get

$$J_0(\lambda a) = 0$$

So λa must be a root of J_0. Then,

$$\lambda = \lambda_n = \frac{\alpha}{a},$$

where α_n is the nth positive zero of J_0. So we can see that:

$$R_n(r) = J_0(\frac{\alpha_n}{a} r), n = 1, 2, ...$$

Using the same λ, we can also see:

$$T_n(t) = A_n \cos c\lambda_n t + B_n \sin c\lambda_n t$$

Utilizing the same superposition principles that we saw with the heat and wave equations, we can write our solution u by:

$$u(r,t) = \sum_{n=1}^{\infty} \left(A_n \cos c\lambda_n t + B_n \sin c\lambda_n t\right) J_0(\lambda_n r)$$

In order to determine the coefficients of this solution, we will need to use **Fourier-Bessel expansions** of a function f, which is seen as follows:

Theorem 4.2.1. [1] *Given a function f that is piecewise smooth on an interval $[0, a]$, then f has a Bessel series expansion of order p on the interval $(0, a)$ given by*

$$f(x) = \sum_{j=1}^{\infty} A_j J_p(\lambda_{pj} x) \tag{4.7}$$

where $\lambda_{p1}, \lambda_{p2}, ...$ are the zeroes of the Bessel function J_p.

Setting $t = 0$, we get,

$$u(r,0) = f(r) = \sum_{n=1}^{\infty} A_n J_0(\lambda_n r),$$

which we can recognize as the Bessel Expansion of f of order $p = 0$. To solve for A_n, we can first multiply both sides by $J_0(\lambda_k r)x$ and integrate term by term on $[0, a]$ The we see:

$$\int_0^a f(x) J_0(\lambda_k x) x dx = \sum_{n=1}^{\infty} A_n \int_0^a J_0(\lambda_n x) J_0(\lambda_k x) x dx$$

We can use the orthogonality properties of J_0 to show that the right side is 0 except for when $k = n$. If we cancel out the zero terms, and use the fact that $\int_0^a J_p^2(\lambda_{p,j}) x dx = \frac{a^2}{2} J_{p+1}^2(\alpha_{p,j})$, where $\lambda_{p,j} = \frac{\alpha_{p,j}}{a}$, then

$$\begin{aligned} A_n &= \frac{\int_0^a f(x) J_0(\lambda_n r) r dr}{\int_0^a J_0^2(\lambda_n r) r dr} \\ &= \frac{2}{a^2 J_1^2(\alpha_n)} \int_0^a f(r) J_0(\lambda_n r) r dr \end{aligned}$$

We can also termwise differentiate our solution u and use the other boundary condition to solve for our other coefficient:

$$u_t(r,0) = g(r) = \sum_{n=1}^{\infty} c\lambda_n B_n J_0(\lambda_n r)$$

Similarly as above, we can see,

$$B_n = \frac{2}{c\alpha_n a J_1^2(\alpha_n)} \int_0^a g(r) J_0(\lambda_n r) r dr$$

Thus, we have all the tools we need to solve a vibrating membrane problem. We will show this with some examples.

Example 4.2.1. *Solve vibrating membrane problem for the given data:* $a = 2$, $c = 1$, $f(r) = 0$, $g(r) = 1$.

Proof. Let us first solve for the coefficients:

$$\begin{aligned}
A_n &= \frac{2}{4J_1^2(\alpha_n)} \int_0^2 (0) J_0(\lambda_n r) r dr \\
&= 0 \\
B_n &= \frac{2}{2\alpha_n J_1^2(\alpha_n)} \int_0^2 J_0(\lambda_n r) r dr \\
&= \frac{1}{\alpha_n J_1^2(\alpha_n)} \left(J_1 \left(\frac{\alpha_n}{2} r \right) r \Big|_0^2 \right) \qquad \text{(by Corollary 4.1.2)} \\
&= \frac{2}{\alpha_n \left(J_1(\alpha_n) \right)}
\end{aligned}$$

Thus, our solution is:

$$u(r,t) = \sum_{n=1}^{\infty} \frac{2}{\alpha_n J_1(\alpha_n)} \sin\left(\frac{\alpha_n}{2} t \right) J_0 \left(\frac{\alpha_n}{2} r \right)$$

□

4.3 Other Orthogonal Functions

Frequently throughout this paper we have discussed orthogonal functions and their uses, however we have not fully defined the concept that we are using. Let us define a real linear space V as a **(real) inner product space** [2] if for any two vectors $u, v \in V$, there is a real number $\langle u, v \rangle \in \mathbb{R}$, that is the inner product of u and v that satisfy the following:

1. $\langle u, v \rangle = \langle v, u \rangle$ for all $u, v \in V$
2. $\langle u + v, w \rangle = \langle u, w \rangle + \langle v, w \rangle$ for all $u, v, w \in V$
3. $\langle \alpha u, v \rangle = \alpha \langle u, v \rangle$ for all $u, v \in V$ and $\alpha \in \mathbb{R}$
4. $\langle v, v \rangle \geq 0$ for all $v \in V$, moreover, $\langle v, v \rangle > 0$ for all $v \neq 0$

We want to consider functions as vectors in a vector space. Just as we "dot" vectors in a $\mathbb{R}^n$ to find the angle between the vectors, consider the "dot product" of two functions f, g, which we will denote as $\langle f, g \rangle$, where

f, g are both defined and continuous on some interval $[0, p]$. We then refer to the **inner product** of f and g by:

$$\langle f, g\rangle = \int_0^p f(x)g(x)dx.$$

Just as with dot products of vectors, we say that **two functions are orthogonal if their inner product is zero**.

We have already seen examples of orthogonal functions with sine, cosine, and Bessel functions. In the following subsection, we will see one more example of these orthogonal functions, which we will use further on in the paper.

4.3.1 Hermite Polynomials

There is another group of functions that is important to study in this exploration into partial differential equations: **Hermite Polynomials**. Like Bessel functions, sine and cosine, Hermite polynomials have interesting expansions and orthogonality properties that we can use to solve partial differential equations. The PDE in question is **Hermite's differential equation of order** n:

$$y'' - 2xy' + 2ny = 0, \qquad -\infty < x < \infty \tag{4.8}$$

If we assume a solution of the form $y = \sum_{m=0}^{\infty} a_m x^m$, we can derive the following relation for the coefficients:

$$a_{m+2} = \frac{2m - 2n}{(m+2)(m+1)} a_m, \qquad m = 0, 1, 2, ...$$

Therefore, all the even a_m can be determined from a_0 and all the odd a_m can be determined by a_1. Using this equation, we see that $a_{n+2} = 0$ so $a_{n+4} = 0$, and so forth. We can see that one solution is a polynomial of degree n. If we set $a_n = 2^n$, we get the **Hermite Polynomial**, $H_n(x)$:

$$H_n(x) = n! \sum_{j=0}^{M} \frac{(-1)^j (2x)^{n-2j}}{j!(n-2j)!} \tag{4.9}$$

where $M = \frac{n}{2}$ if n is even and $M = \frac{n-1}{2}$ if n is odd. As with our other functions, the Hermite polynomials have interesting orthogonality properties.

When the product of two Hermite polynomials are taken and multiplied by a weight function, in this case, e^{-x^2}, we can see the following:

We can derive the first few Hermite polynomials using equation (4.9)

Example 4.3.1.

$$\begin{aligned}
H_0(x) &= 0! \sum_{j=0}^{M} \frac{(-1)^j (2x)^{-2j}}{j!(-2j)!}, M = 0 \\
&= 1 \\
H_1(x) &= 1! \sum_{j=0}^{0} \frac{(-1)^j (2x)^{1-2j}}{j!(1-2j)!} \\
&= 2x \\
H_2(x) &= 2! \sum_{j=0}^{1} \frac{(-1)^j (2x)^{2-2j}}{j!(2-2j)!} \\
&= 2\left(\frac{4x^2}{2} + \frac{-1}{1}\right) \\
&= 4x^2 - 2 \\
H_3(x) &= 3! \sum_{j=0}^{1} \frac{(-1)^j (2x)^{3-2j}}{j!(3-2j)!} \\
&= 6\left(\frac{8x^3}{3!} + \frac{(-1)(2x)}{1}\right) \\
&= 8x^3 - 12x
\end{aligned}$$

Theorem 4.3.1. *For non-negative integers m and n, such that $m \neq n$:*

$$\int_{-\infty}^{\infty} H_m(x) H_n(x) e^{-x^2} dx = 0.$$

If $m = n$:

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

We can also represent the nth Hermite Polynomial with the following **Rodrigues-type formula** [1]:

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \tag{4.10}$$

We will verify this by deriving H_0, H_1, H_2, H_3, using this formula.

Example 4.3.2.

$$\begin{aligned}
H_0(x) &= (-1)^0 e^{x^2} \frac{d^0}{dx^0} e^{-x^2} \\
&= 1 \\
H_1(x) &= (-1)^1 e^{x^2} \frac{d}{dx} e^{-x^2} \\
&= (-1)(-2x) e^{x^2} e^{-x^2} \\
&= 2x \\
H_2(x) &= (-1)^2 e^{x^2} \left(\frac{d^2}{dx^2} e^{-x^2} \right) \\
&= e^{x^2} \left((-2x)^2 e^{-x^2} - 2e^{-x^2} \right) \\
&= 4x^2 - 2 \\
H_3(x) &= (-1)^3 e^{x^2} \left(\frac{d^3}{dx^3} e^{-x^2} \right) \\
&= -e^{x^2} \left((-2x)^3 e^{-x^2} - 8xe^{-x^2} - 4xe^{-x^2} \right) \\
&= 8x^3 + 12x
\end{aligned}$$

We can use equation (4.10) to show the following:

Proposition 4.3.2.

$$H_n(x) = 2xH_{n-1}(x) - H'_{n-1}(x), n = 1, 2, ...$$

Proof.

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

Thus,

$$(-1)^{n-1} e^{-x^2} H_{n-1}(x) = \frac{d^{n-1}}{dx^{n-1}}$$

So,

$$\begin{aligned}(-1)^n e^{-x^2} H_n(x) &= \frac{d}{dx}\left[(-1)^{n-1} e^{-x^2} H_{n-1}(x)\right] \\ &= (-1)^{n-1}\left[(-2x)e^{-x2} H_{n-1}(x) + e^{-x^2} H'_{n-1}(x)\right] \\ &= (-1)^{n-1} e^{-x^2}\left[-2x H_{n-1}(x) + H'_{n-1}(x)\right]\end{aligned}$$

Therefore,

$$H_n(x) = 2x H_{n-1}(x) + H'_{n-1}(x)$$

□

We can also demonstrate the orthogonality of the Hermite Polynomials. For instance, consider:

$$\int_{-\infty}^{\infty} H_1(x) H_2(x) e^{-x^2} dx$$

Example 4.3.3.

$$\begin{aligned}\int_{-\infty}^{\infty} H_1(x) H_2(x) e^{-x^2} dx &= \int_{-\infty}^{\infty} (8x^3 - 4x) e^{-x^2} dx \\ &= 8 \int_{-\infty}^{\infty} x^3 e^{-x^2} dx + \int_{-\infty}^{\infty} (-4) x e^{-x^2} dx\end{aligned}$$

We can break this up to evaluate:

Use Mathematica to find $8 \int_{-\infty}^{\infty} x^3 e^{-x^2} dx,$ *. We can then see the Mathematica input in Listing 4.1:*

Listing 4.1: Mathematica Input

```
Integrate[x^(3)*E^(-x^(2))dx,{x,-Infinity, Infinity }]
```

$$\begin{aligned}8 \int_{-\infty}^{\infty} x^3 e^{-x^2} dx &= 4e^{-x^2}\left(-1 - x^2\right)\Big|_{-\infty}^{\infty} \\ &= 0\end{aligned}$$

.

We can use u substitution to solve $\int\limits_{-\infty}^{\infty} (-4)xe^{-x^2}dx$, *setting* $u = -x^2$, *we get:*

$$\begin{aligned} 2\int e^u du &= 2e^{-x^2}\Big|_{-\infty}^{\infty} \\ &= 0 \end{aligned}$$

Thus,

$$\int\limits_{-\infty}^{\infty} H_1(x)H_2(x)e^{-x^2}dx = 0$$

We will see a use for Hermite polynomials in the next chapter as we look at some applications in quantum physics.

Chapter 5

Schrödinger's Equation

One of the most interesting applications of partial differential equations occurs in the world of quantum physics. Sir Isaac Newton was able to model the motion of most objects, however very small particles, like electrons, were beyond the scope of his work. There is a famous result in quantum physics that states that one cannot be certain of the position and the velocity of a particle at any point in time. As we increase our knowledge about the position of the particle, we decrease our knowledge of the velocity, and vice versa. Since we cannot know exactly the position and velocity with exact precision, physicists began to develop a theory that is based on statistical viewpoints. "This revolutionary theory, known as quantum mechanics, postulates that the position of atomic particles can only be determined with a certain probability" [1].

If we consider a single electron moving along the x-axis, we attach a **probability density function** at a given time t, denoted $\rho(x,t)$, that shows the probability that we will find the electron in a given interval $[a,b]$ at the specified time.. We can calculate this probability as follows:

$$\int_a^b \rho(x,t)dx$$

Another important component to discuss is the **wave function** of the electron, denoted $\psi(x)$, which is a complex-valued function. We can compute the probability density function for the electron by its wave function. More specifically:

$$\rho(x) = |\psi(x)|^2 = \psi(x)\overline{\psi(x)},$$

Where $\overline{\psi(x)}$ is the complex conjugate of $\psi(x)$

We can now begin to discuss the 1D Schrödinger Equation for $\psi(x,t) \in \mathbb{C}$, for position x and time t. We define the **One Dimensional Schrödinger Equation** as:

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{\mu}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi(x), \tag{5.1}$$

Where $\hbar$ is **Planck's constant**, which Einstein used in his explanation of the photoelectric effect, and serves as a fundamental constant in the formulation of quantum mechanics [1]. μ is the mass of the particle, and V is a function for the potential energy of the field in which the particle is located. Notice that V is independent of time.

Once again, we are going to take a separation of variables approach to the solution of this equation. Assume:

$$\psi(x,t) = U(x)T(t)$$

so,

$$i\hbar T'(t)U(x) = \frac{-\hbar^2}{\mu}U''(x)T(t)$$

Example 5.0.4. *Let us examine a classic case in studying Schrödinger's equation: the "particle in a box", i.e.:*

$$V(x) = \begin{cases} 0, & \text{if } a \le x \le b \\ \infty, & \text{otherwise} \end{cases},$$

i.e. the particle can only be found in the box defined by $[a,b]$. The potential outside of the box is sufficiently high that the probability of finding the particle outside of the box is zero. Then $V(x) = 0$ in this equation. For the sake of this example, let us take $[a,b] = [0,L]$, for a constant L. Thus,

$$i\hbar\frac{T'}{T} = \frac{-\hbar^2}{\mu}\frac{U''}{U} = E,$$

where E is the separation constant, then

$$T' = \frac{E}{i\hbar}T = \frac{-iE}{\hbar}T$$

This takes a solution of the form:

$$T = Ae^{\frac{-iEt}{\hbar}} \in \mathbb{C}$$

We can also see that:

$$U'' = -\frac{2\mu E}{\hbar^2}U$$

And since $E > 0$, and we can define $\lambda = \sqrt{\frac{2\mu E}{\hbar^2}}$,

$$U(x) = \sin \lambda x$$

Since $U(L) = 0$, then $\sin \lambda L = 0$, or $\lambda L = n\pi$, for $n = 1, 2, \ldots$. So we can see that

$$E = E_n = \frac{n^2\pi^2\hbar^2}{2\mu L^2}$$

for $n = 1, 2, \ldots$.

Therefore, we get a solution to the one dimensional Schrödinger equation:

$$\psi_n(x,t) = Ae^{\frac{-iE_n t}{\hbar}} \sin \frac{n\pi}{L}x$$

In general, we get:

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x,t)$$

We can use Mathematica to graph various solutions to the particle in a box problem. In figure (5.1) we can see the both the real and imaginary parts of $\psi_1(x,t)$, as well as the probability density function $|\psi_1(x,t)|^2$ and see how these components evolve over time. We can see that the real and imaginary components of the wave function ψ_1 evolve and change with time, but the probability function is independent of time.

We can also see an example in which the probability function is not independent of time. This occurs when we look at the superposition of two of these states: $\frac{1}{\sqrt{2}}\psi_1(x,t) + \frac{1}{\sqrt{2}}\psi_2(x,t)$. We can see this in figure (5.2). We can see that as t changes, not only do the real and imaginary parts of the equation change, but the probability density function evolves over time as well.

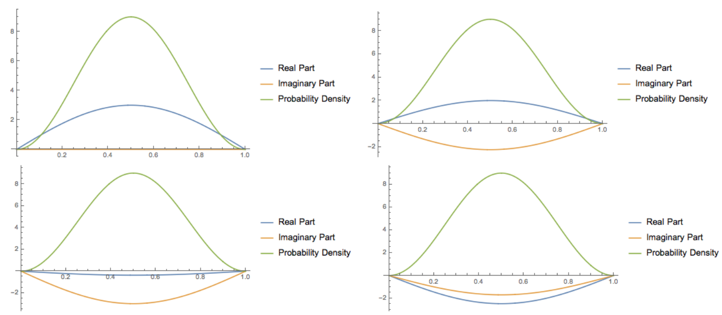

Figure 5.1: Plotting how $\psi_1(x,t)$ changes with time

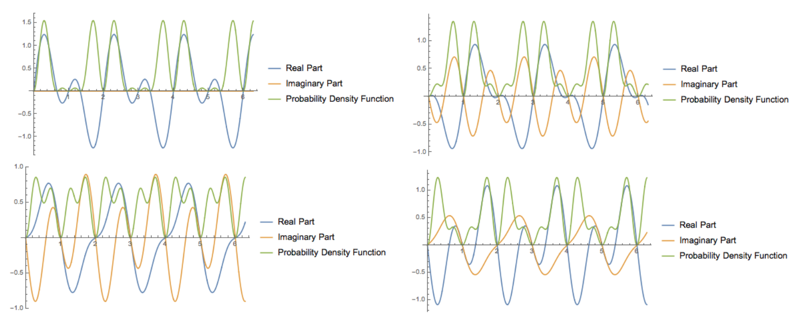

Figure 5.2: Plotting how $\frac{1}{\sqrt{2}}\psi_1(x,t) + \frac{1}{\sqrt{2}}\psi_2(x,t)$ changes with time

5.1 The Quantum Harmonic Oscillator

The **quantum harmonic oscillator**, which is an analog to the spring-mass system in quantum mechanics. We model the small vibrations of a particle of mass μ that moves along the x-axis under a potential force $V(x) = \frac{1}{2}kx^2$, where k is a constant. Using this potential, Schrödinger's equation becomes:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}\psi + \frac{1}{2}kx^2\psi, \tag{5.2}$$

where $\psi = \psi(x,t)$ is the unknown wave function. We want to solve this with a given initial wave function

$$\psi(x,0) = f(x) \tag{5.3}$$

The separate equations now consist of the following:

$$T' = -\frac{i}{\hbar}ET$$

and the one dimensional time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2\mu}u'' + \frac{1}{2}kx^2u = Eu \tag{5.4}$$

We will show how Hermite's differential equation relates to equation (5.4):

Recall equation (4.8) and substitute $\phi(x) = e^{-\frac{x^2}{2}}y(x)$ to yield:

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

We have seen that $H_n(x)$ for $n = 1, 2, ...$ is a solution for $y'' - 2xy' + 2ny = 0$. Thus $e^{-\frac{x^2}{2}}H_n(x)$ is a solution for the above equation.

We can also show that $\phi_m(x)$ and $\phi_n(x)$ are orthogonal for $m \neq n$:

$$\int_{-\infty}^{\infty} \phi_m(x)\phi_n(x)dx = \int_{-\infty}^{\infty} e^{-\frac{x^2}{2}} H_m(x) e^{-\frac{x^2}{2}} H_n(x)dx$$
$$= \int_{-\infty}^{\infty} H_m(x)H_n(x)e^{-x^2}dx = 0$$

as Hermite polynomials are orthogonal functions, with respect to weight e^{-x^2}. Similarly, we state that

$$\int_{-\infty}^{\infty} [\phi_m(x)]^2 dx = \int_{-\infty}^{\infty} H_m^2(x)e^{-x^2}dx = 2^m m!\sqrt{\pi}$$

as it can be shown that $\int_{-\infty}^{\infty} H_n^2(x)e^{-x^2}dx = 2^n n!\sqrt{\pi}$[1].

We say that a function f is **normalizable** if f tends to 0 at infinity, and $|f|^2$ has a finite integral over the defined space. Then we can see that the differential equation

$$\phi'' + (\lambda - x^2)\phi = 0 \tag{5.5}$$

has normalizable solutions on $(-\infty, \infty)$ only when $\lambda = 2n+1$ for $n = 1, 2, ...$ In this instance, our solutions are Hermite polynomials.

Now, define $x = \sqrt{\frac{\hbar}{\mu\omega}}s$, where $k = \mu\omega^2$, and apply the change of variables to equation (5.4). We will use this change of variable to produce a solution to the quantum harmonic oscillator problem. Then:

$$-\frac{\hbar^2}{2\mu}u'' + \frac{1}{2}kx^2u = Eu$$

becomes, as $\frac{d}{dx} = \frac{d}{dx}\frac{dx}{ds}$:

$$-\frac{\hbar^2}{2\mu}\frac{1}{\left(\sqrt{\frac{\hbar}{\mu\omega}}\right)^2}\frac{\partial^2 u}{\partial s^2} + \frac{1}{2}(\mu\omega^2)\frac{\hbar}{\mu\omega}s^2 u = Eu$$

$$\left(-\frac{\hbar}{2\mu}\right)\left(\frac{\mu\omega}{\hbar}\right)\frac{\partial^2 u}{\partial s^2} + \frac{1}{2}(\mu\omega^2)\frac{\hbar}{\mu\omega}s^2 u = Eu$$

$$2Eu + \hbar\omega\frac{\partial^2 u}{\partial s^2} - \hbar\omega s^2 u = 0$$

$$\frac{2E}{\hbar\omega}u + \frac{\partial^2 u}{\partial s^2} - s^2 u = 0$$

So we see that the equation has been transformed to:

$$\frac{\partial^2 u}{\partial s^2} + \left(\frac{2E}{\hbar\omega} - s^2\right)u = 0$$

Thus, using the conclusion we made from equation (5.5), we see that the solutions to this equation are $E = E_n = \hbar\left(n + \frac{1}{2}\right), n = 0, 1, 2, ...$, and each E_n has the following solution:

$$u_n(x) = e^{-\frac{\mu\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{\mu\omega}{\hbar}}x\right), n = 0, 1, 2, ...$$

We can use this result in conjunction with our product solution to the one-dimensional Schrödinger equation to show that the product solutions of equation (5.2) are:

$$\psi_n(x,t) = A_n e^{-iE_n t/\hbar}u_n = A_n e^{-iE_n t/\hbar}e^{-\frac{\mu\omega x^2}{2\hbar}}H_n\left(\sqrt{\frac{\mu\omega}{\hbar}}x\right)$$

One last time, using our motivation of the superposition principle, we see that the general solution to the quantum harmonic oscillator is:

$$\begin{aligned}\psi(x,t) &= \sum_{n=0}^{\infty} A_n e^{-iE_n t/\hbar}e^{-\frac{\mu\omega x^2}{2\hbar}}H_n\left(\sqrt{\frac{\mu\omega}{\hbar}}x\right)\\ &= e^{-\frac{\mu\omega x^2}{2\hbar}}\sum_{n=0}^{\infty} A_n e^{-iE_n t/\hbar}H_n\left(\sqrt{\frac{\mu\omega}{\hbar}}x\right)\end{aligned}$$

To solve for A_n, we will use the following theorem, recalling $\psi(x,0) = f(x)$. Then, $\psi(x,0) = f(x) = \sum_{n=1}^{\infty} A_n u_n(x)$, for some normal mode solution $u_n(x)$. We use orthogonality in the usual way to show:

Theorem 5.1.1.

$$A_n = \int_{-\infty}^{\infty} f(x)u_n(x)dx / \int_{-\infty}^{\infty} u_n^2(x)dx$$

[1]

We know from previously that:

$$\int_{-\infty}^{\infty} u_n^2(x)dx = \sqrt{\frac{\hbar}{\mu\omega}} 2^n n! \sqrt{\pi}$$

Thus,

$$\begin{aligned} A_n &= \sqrt{\frac{\mu\omega}{\hbar}} \frac{1}{2^n n! \sqrt{\pi}} \int_{-\infty}^{\infty} f(x)u_n(x)dx \\ &= \sqrt{\frac{\mu\omega}{\hbar}} \frac{1}{2^n n! \sqrt{\pi}} \int_{-\infty}^{\infty} f(x)e^{-\frac{\mu\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{\mu\omega}{\hbar}} x\right) dx. \end{aligned}$$

Example 5.1.1. *Take* $\frac{\mu\omega}{\hbar} = 1$ *and consider the initial value problem given by equations (5.2)-(5.3), where* $f(x) = Ae^{-\frac{x^2}{2}}$*.*

Proof. We first need to normalize $f(x)$. This is known to be when $A = \frac{1}{\sqrt{\pi}}$ Then we can solve for A_n by:

$$\begin{aligned} A_n &= \frac{1}{2^n n! \sqrt{\pi}} \int_{-\infty}^{\infty} f(x)e^{-x^2/2} H_n(x)dx \\ &= \frac{1}{2^n n! \pi} \int_{-\infty}^{\infty} e^{-x^2} H_n(x)dx \\ &= \frac{1}{2^n n! \pi} \int_{-\infty}^{\infty} e^{-x^2} H_0(x)H_n(x)dx, \end{aligned}$$

which is 0 for $n \neq 0$, but when $n = 0$, $A_0 = \frac{1}{2^0(0)!\pi}(2^0(0)!\sqrt{\pi}) = \frac{1}{\sqrt{\pi}}$. Thus,

$$\begin{aligned} \psi(x,t) &= e^{-\frac{x^2}{2}} \left(\frac{1}{\sqrt{\pi}}\right) e^{-iE_0 t/\hbar} H_0(x) \\ &= \frac{1}{\sqrt{\pi}} e^{-\frac{x^2}{2}}. \end{aligned}$$

□

Bibliography

[1] N. Asmar, *Partial Differential Equations with Fourier Series and Boundary Value Problems*, 2nd ed., Pearson Education, Upper Saddle River, NJ, 2005.

[2] Y. Pinchover and J. Rubinstein, *An Introduction to Partial Differential Equations*, 1st ed., Cambridge University Press, University Press, Cambridge, 2005.

[3] J. David Logan, *Applied Partial Differential Equations*, 1st ed., Springer-Verlag, New York, New York, 1998.