Fourier Transforms and Numerically Approximating PDE's

Cody Morgan, Advised by Dr. Jonathan L. Mitchell

Stephen F. Austin State University, Nacogdoches, TX

Abstract

The Fourier Transform is a mathematical tool used in many scientific disciplines that converts an input of a temporal (time) signal to a set of frequencies, which can then be used for analysis. There are three main topics of which this project focuses on; we will utilize the Fourier Transform (FT) to **process signals containing noise**, introduce a special class of mathematical equations known as **partial differential equations** (PDEs), and hone in on a PDE in the form of the *Schrödinger Equation*, which is a well-established law in the field of **quantum mechanics**. The classical mechanics analogue for the Schrödinger Equation is Newton's 2nd Law of Motion; both are known to be the cornerstones in their respective branches of physics and aim to mathematically describe the motion of different objects/systems. Hence, their significance is the motivation for this research.

Fourier Transform, Analytically and Numerically

- The Fourier Transform (FT) of a wave form $f(t)$ is defined as

$$F(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(t)e^{-i\omega t}dt \tag{1}$$

This integral transform is commonly applied in many scientific contexts including signal processing, quantum mechanics, image reconstruction, and others. Mathematically, the FT is a function of angular frequency, ω, whose output indicates frequencies that are dominant in the wave form $f(t)$. In **Figure 1** (left), we observe a simple linear wave form $f(t)$. Using **Equation 1**, we determine its FT to be the frequency function given by **Equation 2** and is shown in **Figure 1** (right).

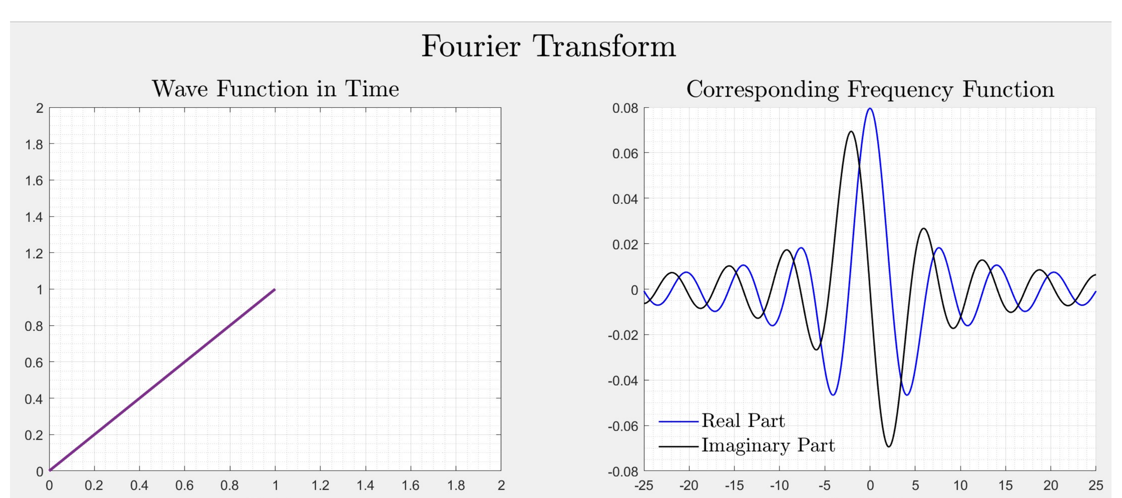


Figure 1. A Transformed Signal

$$F(\omega) = \frac{1}{2\pi}\int_{0}^{1} te^{-i\omega t}dt = \frac{1}{2\pi}\left(\frac{e^{-i\omega}-1}{\omega^2} - \frac{e^{-i\omega}}{i\omega}\right) \tag{2}$$

Because this is a complex function, one can plot both real and imaginary parts or perhaps the modulus of the FT in order gain a visual understanding of the dominant frequencies at play in the original signal. However, generating these calculations for more complex wave forms becomes cumbersome or even impossible to do so by hand, so numerical methods are implemented for efficiency.

- **NUMERICAL APPROXIMATION USING *fft*:** MATLAB's Fast Fourier Transform (**fft**) function can be used to computationally transform temporal functions, which is especially useful when the signal contains noise. The **fft** function works by taking on multiple parameters that are passed as inputs, such as: the length of the signal, sampling frequency/period, and number of plot points. An example of a numerical Fourier Transform applied to two different noisy time signals is shown in **Figure 2**.

The remnants of the transform are varying frequencies of which the original signal was comprised. These values can then be plotted and often indicate a Dirac delta function, having spikes at locations of the dominant frequency values from the original signal.

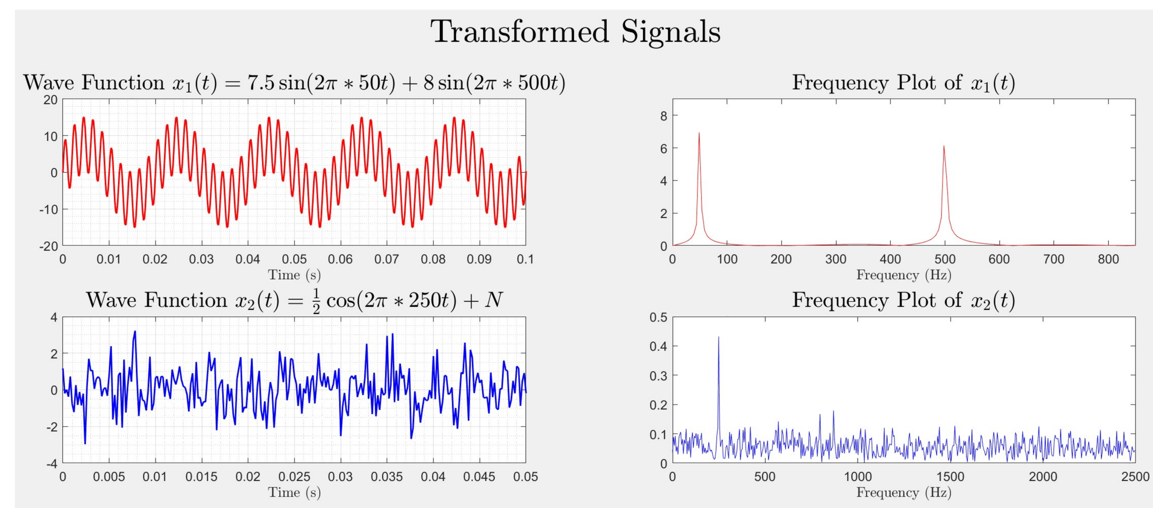


Figure 2. Noisy Signals and Their Dominant Frequencies

In **Figure 2**, $x_1(t)$ (top left) is the sum of two different sinusoids; $x_2(t)$ (lower left) is a sinusoid with additive noise, N, which is a random variable with standard normal distribution. This was computed using MATLAB's `randn` function, giving it its jagged appearance.

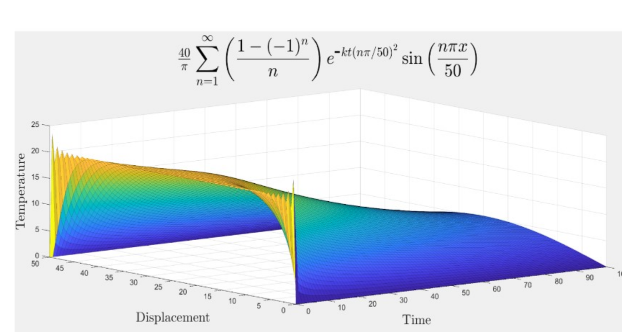
If the original signal is not known but the frequency signal has been established, an Inverse FT could be used to recover (or approximately recover) the original signal by reestablishing the time dependency. In fact, both the FT and its inverse can be utilized when numerically solving certain partial differential equations; this is one of the many applications of the FT other than that of signal processing.

Elementary Partial Differential Equations

- WHY ARE THEY IMPORTANT? Often times, partial differential equations (PDEs) are used to model physical phenomena. Two examples of such expressions, the *heat equation* and *wave equation*, are subjects of particular interest when first studying PDEs because of their clear connection to physical situations and elegant solutions.
- COMPARING THE METHODS OF GENERATING SOLUTIONS: The two most basic forms of PDEs, as mentioned before, are the *heat equation* and *wave equation*, which take the form

$$\frac{\partial u}{\partial t} = k\left(\frac{\partial^2 u}{\partial x^2}\right) \quad \text{and} \quad \frac{\partial^2 u}{\partial t^2} = a^2\left(\frac{\partial^2 u}{\partial x^2}\right), \tag{3}$$

respectively. The conceptualization of the *heat equation* is modeling a 1-D rod heating up or cooling off with a specified initial temperature, where k is the thermal diffusivity. Furthermore, a represents the velocity of propagation in the *wave equation*, which models a vibrating string with a specified initial shape. To analytically generate solutions to these PDEs, the *separation of variables* method is implemented, followed by applying a *Fourier Series* and the boundary conditions (BCs) to generate a particular solution. An example of a calculated solution is shown below, where the surface is generated by a 100 iterations of the infinite sum below.

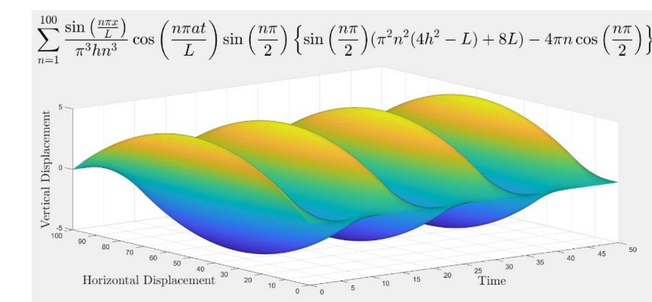


	Constant IC	Piecewise Linear IC
Low Diffusivity		
High Diffusivity		

Figure 3. Different Approaches to *Heat Equation* Problems

The plotted surfaces are visual representations of how a metal rod might cool off in time from an initial temperature. It can be seen that the "height" of the surface represents the temperature at the corresponding location along the rod in time. The surface in **Figure 3** has boundary conditions that are equal to 0°, as if the ends of the metal rod were submerged in an ice bath. MATLAB's `pdepe` function was utilized to be able to solve the heat equation with varying BCs, ICs, and complexity more efficiently, as shown by the videos linked in **Figure 3** on the right.

On the other hand, the *wave equation* is a bit more mathematically involved; four conditions – two initial and two boundary – specify the wave's starting shape and speed before it's sent into propagation. In a similar fashion, an exact solution and several computational ones are shown in **Figure 4** below.



	Harmonic IC	Other IC
Fixed Ends		
Varying Ends		

Figure 4. Different Solutions to *Wave Equation* Problems

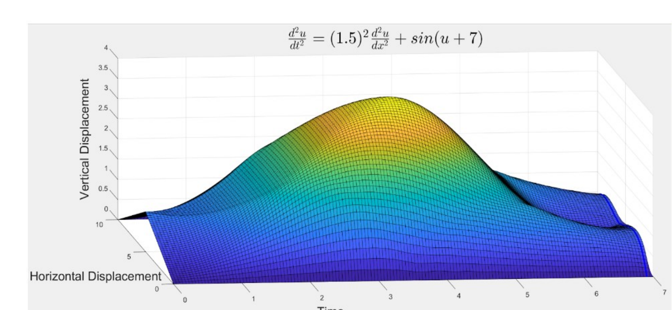
We used a *center-space difference* approach for numerical solutions to the wave equation, given by

$$u_n^{j+1} = s\left(u_{n+1}^j + u_{n-1}^j\right) + 2(1-s)u_n^j - u_n^{j-1} \tag{4}$$

where the subscript is the space index, the superscript is the time index, and $s = (a\Delta t/\Delta x)^2$, which must be less than unity for the algorithm to be stable. We also applied this method to the *Klein-Gordon Equation*, which is a PDE that takes the form

$$\frac{d^2u}{dt^2} = a^2\left(\frac{d^2u}{dx^2}\right) + F(u). \tag{5}$$

where F can be any elementary - often nonlinear - function of u. The MATLAB code will populate a matrix u as it runs through the *center-space difference method* algorithm that was developed. For accessibility, a specific example is illustrated below, using $a = 1.5$ and $F(u) = \sin(u+7)$ with a piecewise linear IC.



	Quadratic IC	Sinusoidal IC
Fixed Ends		
Free Ends		

Figure 5. Numerical Approximations to Solutions for the Klein-Gordon Equation

Quantum Mechanics

- **Understanding the Equation:** As it was previously mentioned, Schrödinger's *Wave Equation* is the quantum analogue to Newton's Second Law of Motion; *Schrödinger's Time-Dependent Equation*, shown below, exists as a PDE (hence, its relevance to this study) while its ODE and time-independent counterpart, **Equation 7**, is derived by applying a *separation of variables*.

$$\left(\frac{-\hbar^2}{2m}\right)\frac{\partial^2\Psi}{\partial x^2} + U(x)\Psi(x,t) = i\hbar\frac{\partial\Psi}{\partial t} \tag{6}$$

$$\left(\frac{-\hbar^2}{2m}\right)\frac{d^2\psi}{dx^2} + U(x)\psi(x) = E\psi(x) \tag{7}$$

Here, $\hbar$ is the reduced Planck's Constant, m is the mass of the particle, $U(x)$ is a potential function, E is the quantized energy of the particle, $i = \sqrt{-1}$, and, most importantly, $\Psi(x,t)$ is the wave function for which we desire a solution. To fully understand the importance of this equation and its applications, the coexisting principles of quantum mechanics ought to be understood.

One of the most important principles tied to quantum mechanics is **wave-particle duality**, which is the fact that particles can act similarly to point masses or as waves, depending on how they are observed.

Another key basis of quantum is that **it is impossible to know exactly both a particle's location and velocity at the same time, which is summarized by *Heisenberg's Uncertainty Principle*** (HUP). It is clear that $\Psi(x,t)$ is very important, given that it is the sought-after wave function in the Schrödinger PDE, but what does it tell us? As it turns out, Ψ itself has no physical significance; as required by HUP, **the information that can be known about the particle's motion comes in the form of a probability.** This is summarized by the proceeding relations.

$$P(x)dx = |\Psi(x,t)|^2 dx \qquad \text{and} \qquad \int_{-\infty}^{\infty}|\Psi(x,t)|^2 dx = 1 \tag{8}$$

These show that the square modulus of Ψ is equal to the **probability density** of the particle in question. In other words, finding a solution for Ψ can then yield a probability function that guarantees that the particle has 100% expectancy of existing in all of the possible x values. Once physical constraints have been met, an expectancy (percent) value for the particle's location within a finite range can be calculated using the same integral as above with appropriate limits of integration.

- **The Fundamental Problem of Quantum Mechanics**: Given a physical scenario (like the one shown in **Figure 6**) it is desired to find the wave function for a propagating particle. In this example, the particle will never have enough energy to overcome the infinite potential so it is forever confined to the box; hence, the boundary conditions are $\Psi(0,t) = 0$ and $\Psi(L,t) = 0$. Furthermore, since the wave function has a strong connection to probability, it must be well-behaved by obeying the following conditions.

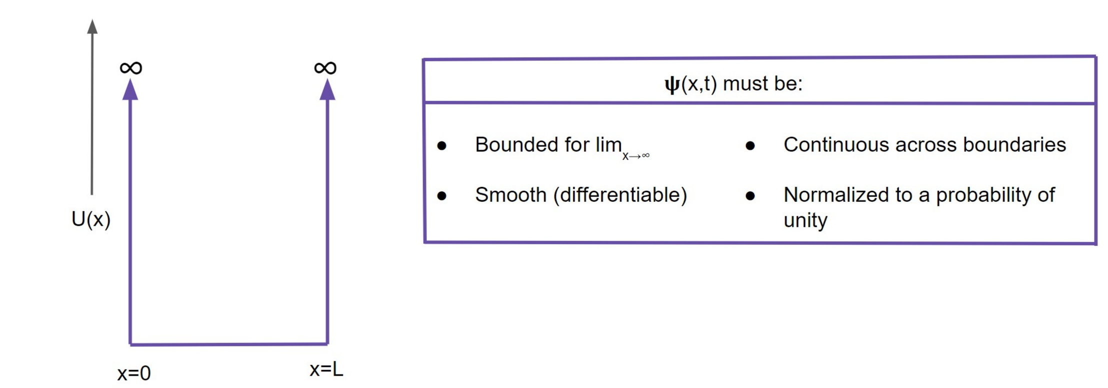


Figure 6. The Infinite Square Well Problem, a Particle in a Box

For this example, there exist no forces within the region inside the box, so we consider the electron to be a *free particle*; this simplifies the PDE, given that $F = -\frac{dU(x)}{dx} = 0$. Once all the conditions and physical constraints have been met, the solution becomes

$$\Psi_n(x,t) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)e^{-\frac{iEt}{\hbar}}, \quad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}. \tag{9}$$

It is important to note that the square moduli of the solutions $\psi(x)$ (referred to as stationary states) and $\Psi(x,t)$ represent the same probability distribution.

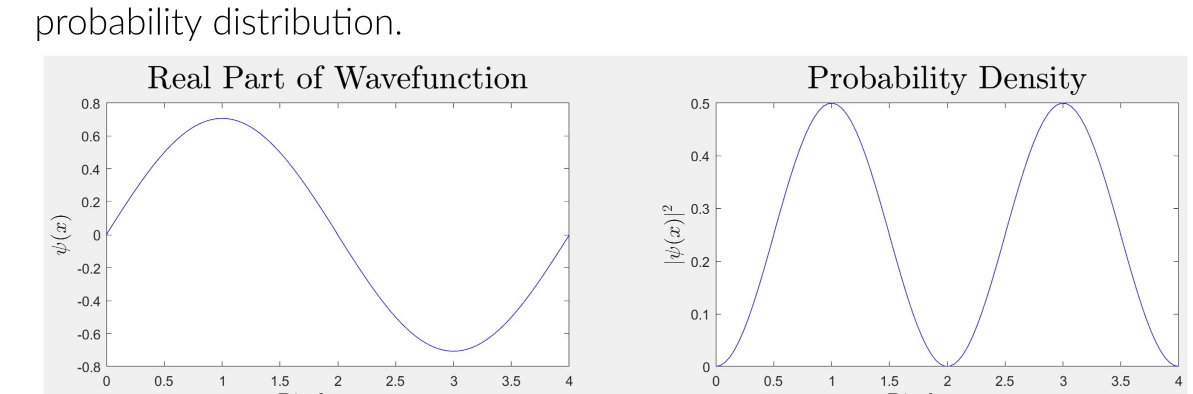


Figure 7. 1st Excited State for an Electron in an Infinite Square Well (n=2)

Future Work

- Additional numerical approaches, such as **spectral methods**, can be applied to problems of higher complexity and would use the Fourier Transform and its inverse to generate solutions to such PDEs
- Specifically, we hope to develop MATLAB code that can generate numerical approximations to solutions of the **Cubic Non-Linear Schrödinger Equation**, which takes the form $i\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} + \lambda|u|^2u = 0$. Solutions to equations of this type are called **solitons** and are relevant to many types of nonlinear applications.

CONTACT
Cody Morgan
SFASU Dept. of Physics, Engineering, & Astronomy
Morganca1@jacks.sfasu.edu

REFERENCES

1. Advanced Engineering Mathematics, Zill & Wright, Jones & Bartlett Learning, 2014
2. Elementary Applied Partial Differential Equations, Haberman, Richard, Prentice-Hall, 1998
3. Solitons: an Introduction, Drazin & Johnson, Cambridge University Press, 1989
4. Modern Physics, Serway, Moses, and Moyer, David Harris, 2019

ACKNOWLEDGEMENTS

This research was made possible by the Stephen F. Austin State University SURE program and the Department of Mathematics and Statistics, from whom additional funding was received. All graphs and surfaces were plotted in MATLAB 2022.
A special thank you to Dr. Jonathan Mitchell, my research advisor, mentor, and friend.