Abstract

The Schrodinger equation is solved by using the split step method,

1 Introduction

2 Schrodinger Equation

3 Fourier Analysis

Fourier analysis plays an important role in the field of science and engineering, it is a subject area which grew from the study of Fourier series. It is named after Joseph Fourier, who showed that representing a function by a trigonometric series greatly simplifies the study of heat propagation. Fourier analysis involves decomposing a function into simpler pieces, the process itself is called a Fourier transform. But before a function (usually a signal) decomposes into simpler functions, it has to be represented first, by using Fourier series to present any periodical function in terms of sine and cosine, which is defined as:

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos(n\frac{2\pi}{T}t) + b_n sin(n\frac{2\pi}{T}t)$$

$$a_0 = \frac{2}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} f(t)dt$$

$$a_n = \frac{1}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} f(x)\cos nxdx$$

$$b_n = \frac{1}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} f(x)\sin nxdx$$

a_0, a_n and b_n are called the Fourier co-efficients of f.

3.1 Derivation of the Fourier Transform

Fourier transform is a generalization of the complex Fourier series in the limit as $T \to \infty$. Using the following trigonometric identity one can simplify the sines and cosines of the Fourier series in terms of exponentials,

$$\cos(2\pi\omega_f) = \frac{e^{2\pi\omega_f t} + e^{-2\pi\omega_f t}}{2}$$

$$\sin(2\pi\omega f) = \frac{e^{2\pi\omega f t} - e^{-2\pi\omega_f t}}{2}$$

the Fourier series becomes,

$$f(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[\left(\frac{a_n}{2} + \frac{b_n}{2i} \right) e^{in\omega_f t} + \left(\frac{a_n}{2} - \frac{b_n}{2i} \right) e^{-in\omega_f t} \right]$$

which can be written as,

$$f(t) = \sum_{n=1}^{\infty} C_n e^{2\pi int}$$

In this form the coefficients C_n are complex numbers. And we can solve it with a direct approach. Lets take the coefficient C_k for some fixed k. We can isolate it by multiplying both sides by $e^{-2\pi ikt}$:

$$e^{-2\pi ikt} f(t) = e^{-2\pi ikt} \sum_{n=-N}^{N} C_n e^{-2\pi int}$$

$$= ... + e^{-2\pi ikt} C_k e^{-2\pi ikt} + ... = ... + C_k + ...$$

thus

$$C_k = e^{-2\pi ikt} f(t) - \sum_{n=-N, n\neq k}^{N} C_n e^{-2\pi ikt} e^{2\pi int}$$

$$= e^{-2\pi ikt} f(t) - \sum_{n=-N, n\neq k}^{N} C_n e^{2\pi i(n-k)t}$$

The coefficient C_k is pulled out, but the expression on the right involves all the other unknown coefficients. Another idea is needed, and that idea is integrating both sides from 0 to 1. Just as in calculus, we can evaluate the integral of a complex exponential by:

$$\int_0^1 e^{2\pi i(n-k)} dt = \frac{1}{2\pi i(n-k)} e^{2\pi i(n-k)} \Big|_{t=0}^{t=1}$$

$$= \frac{1}{2\pi i(n-k)} \left(e^{2\pi i(n-k)} - e^0 \right) = \frac{1}{2\pi i(n-k)} (1-1)$$

Note that $n \neq k$ is needed here. Since the integral of the sum is the sum of the integrals, and the coefficients C_n come out of each integral, all of the terms in the sum integrate to zero and we have a formula for the k-th coefficient:

$$C_k = \int_0^1 e^{-2\pi ikt} f(t) dt$$

3.2 Convolution

3.3 Discrete Fourier Transform

3.4 Fast Fourier Transform

4 Method

5 Results

6 Summary