Numerical Solutions to the Time Dependent Schrodinger Equation for the Harmonic Oscillator Potential

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Abstract

This study investigates the procedure for the solution of the Time Dependent Schrodinger equation in one dimension for the harmonic oscillator potential using the finite difference method. Analytical solutions are notoriously hard thus numerical solutions were employed in the Scilab language. The real and the imaginary parts of the schrodinger equation were solved separately on a grid, and the results were visualized in plots.

1 Introduction

The Time Dependent Schrodinger equation is the centeral entity in Quantum Mechanics. It governs the time evolution of a quantum wave function, which is the state of a particle in Quantum Mechanics. The Time Independent version, which was solved earlier, is a special case of this one. The numerical solutions were implemented by modifying the Heat Equation code created earlier, as the Time Dependent Schrodinger Equation is a variant of the Heat Equation. The Numerical solutions were implemented in the Scilab language, because it makes working with matrices much easier than alternatives. Similar to the heat equation, the problem was broken down into solving on a 2 dimensional grid, but this time solutions for the real and the imaginary parts of the wave function had to be done simultaneously. The algorithm employed for this solution was exactly the same as the Heat Equation, refer to that paper for more information.

2 Results and Discussions

Let us begin our discussion with the mathematical form of the one dimensional time dependent schrodinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t) \tag{1}$$

To proceed with the numerical solution, we will have to replace both the second an the first derivatives with their appropriate finite approximations. Since there are multiple finite approximations available, we will use the following ones that had produced the accurate results before:

$$\frac{\partial^2}{\partial x^2} f(x,t) = \lim_{\Delta x \to 0} \frac{f(x+\Delta x, t) - 2f(x,t) + f(x-\Delta x, t)}{(\Delta x)^2} \tag{2}$$

$$\frac{\partial}{\partial t} f(x,t) = \lim_{\Delta t \to 0} \frac{f(x, t+\Delta t) - f(x,t)}{\Delta t} \tag{3}$$

As we could tell by looking at the form of the Time Dependent Schrodinger equation, The wave function ψ had to be complex. We are equating an imaginary number on the right hand side to a real number on the left hand side, and the only way the two sides can be equal is if either both are zero or the wave function is complex. Solving a literally complex partial differential equation on a computer is going to be messy so we will break up the equation into two, one for each the real and the imaginary parts.

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}[\psi_r + i\psi_i] + V(x)[\psi_r + i\psi_i] = i\hbar\frac{\partial}{\partial t}[\psi_r + i\psi_i] \tag{4}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_r + V(x)\psi_r = -i\hbar\frac{\partial}{\partial t}\psi_i \tag{5}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_i + V(x)\psi_i = i\hbar\frac{\partial}{\partial t}\psi_r \tag{6}$$

$$I_x^{t+1} = I_x^t - \frac{V_x R_x \Delta t}{\hbar} + \frac{\hbar \Delta t}{2m(\Delta x)^2}(R_{x-1}^t - 2R_x^t + R_{x+1}^t) \tag{7}$$

$$R_x^{t+1} = R_x^t + \frac{V_x I_x \Delta t}{\hbar} - \frac{\hbar \Delta t}{2m(\Delta x)^2}(I_{x-1}^t - 2I_x^t + I_{x+1}^t) \tag{8}$$

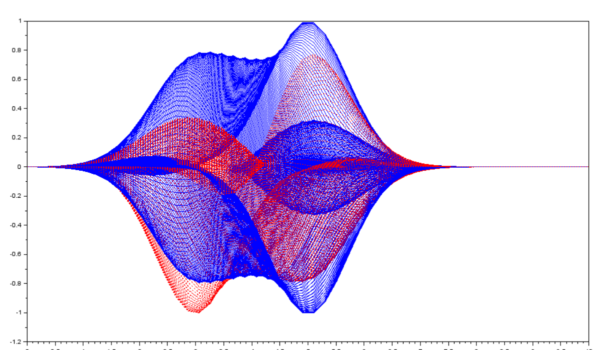

Figure 1: The red part gives the imaginary solution while the blue part the real one.