Numerical Solutions to the Time-Independent Schrodinger Equation for the Harmonic Oscillator Potential

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[*]www.github.com/dominuszain/TimeIndependentSchrodingerEquation/tree/main

Abstract

In this study, we solved the time-independent schrodinger equation by substituting equivalent forms for the single and double derivative operators. The resulting expression was converted to a matrix eigenvalue problem, and solved by computing the eigenvalues and eigenvectors numerically. All the calculations and plots were done in the scilab language.

1 Introduction

The time-independent schrodinger equation is used to find the allowed wave functions for a quantum system and their corresponding energies. The time-dependence can be later added by multiplying this solution with the time evolution operator. Analytical solutions of even moderately complex quantum systems are notoriously hard, thus numerical methods are employed. For the numerical computations, the Scilab language and the Scilab interpreter was used. The reasons for this particular choice were that the software package had a wide variety of built-in functions that would significantly reduce the implimentation time, and the fact that the software package is open-source and cross-platform.

2 Results and Discussions

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

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x) \tag{1}$$

To proceed with the numerical solution, we will have to replace the second derivative $\frac{d^2}{dx^2}$ with it's corresponding finite approximation. The choice of substitution will be done keeping in mind the transformation to a matrix eigenvalue problem. We will use the following substitution for the second derivative:

$$\frac{d^2}{dx^2}f(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} \tag{2}$$

Now making this substitution into the time-independent schrodinger equation would result in the following expressions:

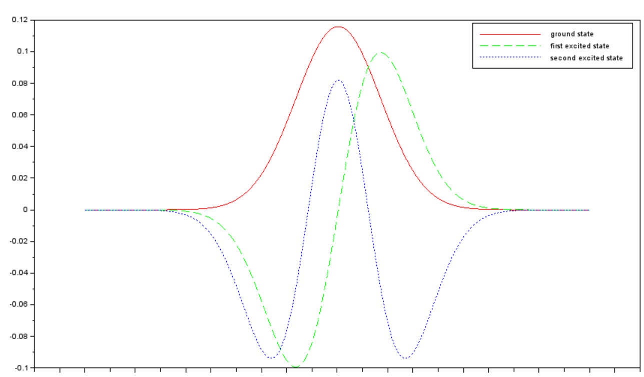
$$-\frac{\hbar^2}{2m}\left(\frac{\psi(x_{i+1}) - 2\psi(x_i) + \psi(x_{i-1})}{h^2}\right) + V(x_i)\psi(x_i) = E\psi(x_i) \tag{3}$$

$$\left(2 + \frac{2mh^2V(x_i)}{\hbar^2}\right)\psi(x_i) - \psi(x_{i+1}) - \psi(x_{i-1}) = \frac{2mh^2E}{\hbar^2}\psi(x_i) \tag{4}$$

Now, the corresponding matrix for this expression would be:

$$\begin{pmatrix} 2+\frac{2mh^2V(x_1)}{\hbar^2} & -1 & 0 & 0 & 0 & \cdots \\ -1 & 2+\frac{2mh^2V(x_2)}{\hbar^2} & -1 & 0 & 0 & \cdots \\ 0 & -1 & 2+\frac{2mh^2V(x_3)}{\hbar^2} & -1 & 0 & \cdots \\ 0 & 0 & -1 & 2+\frac{2mh^2V(x_4)}{\hbar^2} & -1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} |\Psi\rangle = \frac{2mh^2E}{\hbar^2}|\Psi\rangle \tag{5}$$

The matrix is always going to be square, and the larger it is, the better the solutions we get. The eigenvalues and eigenvectors of this matrix do infact correspond to the correct solutions. The image of the first three energy state solutions to this problem have been added, and they indeed represent the correct solutions.



3 Appendix

Here I would like to motivate a little where the substitution for the second derivative has come from. We know that the first derivative can be defined in both of the following ways:

$$\frac{d}{dx}f(x) = lim_{h\to 0}\frac{f(x+h)-f(x)}{h} \tag{6}$$

$$\frac{d}{dx}f(x) = lim_{h\to 0}\frac{f(x)-f(x-h)}{h} \tag{7}$$

Both of these definitions are equally correct, but a far more correct expression for the second derivative can be obtained if we apply one of the definitions onto the other. The expression for the second derivative that comes when we apply a definition onto itself does not work in the above problem. It is only when both are used, the eigenvectors and eigenvalues make sense.

$$\frac{d^2}{dx^2} = lim_{h\to 0}\frac{f(x+h)-f(x+h-h)-f(x)+f(x-h)}{h^2} \tag{8}$$

$$\frac{d^2}{dx^2} = lim_{h\to 0}\frac{f(x+h)-2f(x)+f(x-h)}{h^2} \tag{9}$$

In the future, different expressions for the second derivative, which rely on different assumptions for the first derivatives, could be tested to see if they work with the above matrix and calculate values within a tolerable range of error.