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

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Abstract

This study investigates the results of different substitutions for the second derivative of the wave function in solving the time-independent schrodinger equation for the quantum harmonic oscillator potential. A total of two approximations were tested, and it was found out that one worked flawlessly while the other one did not produce the accurate results. The study emphasizes that the choice of estimation for the second derivative can have polarizing impacts on the outputs.

1 Introduction

The time-independent schrodinger equation is used to find the allowed wave functions for a quantum system and their corresponding energy eigenvalues. 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 opensource 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 problem is that there are more than one expressions that

can substitute the second derivative. Let us start with the definition of the derivatives:

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

Applying the operator again for the second time would give us the expression:

$$\frac{d^2}{dx^2}f(x+\frac{h}{2}) = \lim_{h\to 0}\frac{f(x+2h)-2f(x+h)+f(x)}{h^2} \tag{3}$$

Writing the above expression in the index notation would be required for numerical iterations, such that x_{i+n} is equivalent to $x+nh$ where h is the step size. We can get rid of the limit as long as we promise to keep the step size very small.

$$\frac{d^2}{dx^2}f(x_{i+\frac{1}{2}}) = \frac{f(x_{i+2})-2f(x_{i+1})+f(x_i)}{h^2} \tag{4}$$

A step size is the smallest unit of a numerical calciulation. We can only have positive integer multiples of the step size in our calculations. Thus, the term $i+\frac{1}{2}$ will have to be approximated to either just i or $i+1$. Let us proceed with a formulation that keeps it to i and see what results we get.

$$\frac{d^2}{dx^2}f(x_i) = \frac{f(x_{i+2})-2f(x_{i+1})+f(x_i)}{h^2} \tag{5}$$

Now let's make the above substitution into the time-independent schrodinger equation and simplify:

$$-\frac{\hbar^2}{2m}(\frac{\psi(x_{i+2})-2\psi(x_{i+1})+\psi(x_i)}{h^2}) + V(x_i)\psi(x_i) = E\psi(x_i) \tag{6}$$

The above equation can be simplified and factored into the terms of ψ:

$$(-1+\frac{2mh^2V(x_i)}{\hbar^2})\psi(x_i) + 2\psi(x_{i+1}) - \psi(x_{i+2}) = \frac{2mh^2E}{\hbar^2}\psi(x_i) \tag{7}$$

We can convert the above expression into an eigenvalue problem. The matrix applies to the quantum state vector, and results is that quantum state vector being scaled by a constant. Note that for the wave function to be normalizable, we will apply the condition that it vanishes at both positive and negetive infinities i.e. $\psi(-\infty) = \psi(+\infty) = 0$. Thus, the dimensions of the matrix would be $(n-1)\times(n-1)$, where n is the total number of data points. Now our problem has been reduced to simply calculating the eigenvalues and eigenvectors of this matrix. The eigenvectors would give the different states of the wave function while the eigenvalues would give the corresponding energies scaled by some constant. This approach does not produce the accurate results. This discrepency

can be traced back to the substitution we used for the second derivative. For some reason, unknown as of now, this substitution does not seem to work.

$$\begin{pmatrix} -1+\frac{2mh^2V(x_1)}{\hbar^2} & 2 & -1 & 0 & 0 & \cdots \\ 0 & -1+\frac{2mh^2V(x_2)}{\hbar^2} & 2 & -1 & 0 & \cdots \\ 0 & 0 & -1+\frac{2mh^2V(x_3)}{\hbar^2} & 2 & -1 & \cdots \\ 0 & 0 & 0 & -1+\frac{2mh^2V(x_4)}{\hbar^2} & 2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} |\Psi\rangle = \frac{2mh^2E}{\hbar^2}|\Psi\rangle \tag{8}$$

Now let's proceed with the other formulation that approximates $i+\frac{1}{2}$ to $i+1$. The expression for the second derivative reduced to the following:

$$\frac{d^2}{dx^2}f(x_{i+1}) = \frac{f(x_{i+2})-2f(x_{i+1})+f(x_i)}{h^2} \tag{9}$$

$$\frac{d^2}{dx^2}f(x_i) = \frac{f(x_{i+1})-2f(x_i)+f(x_{i-1})}{h^2} \tag{10}$$

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

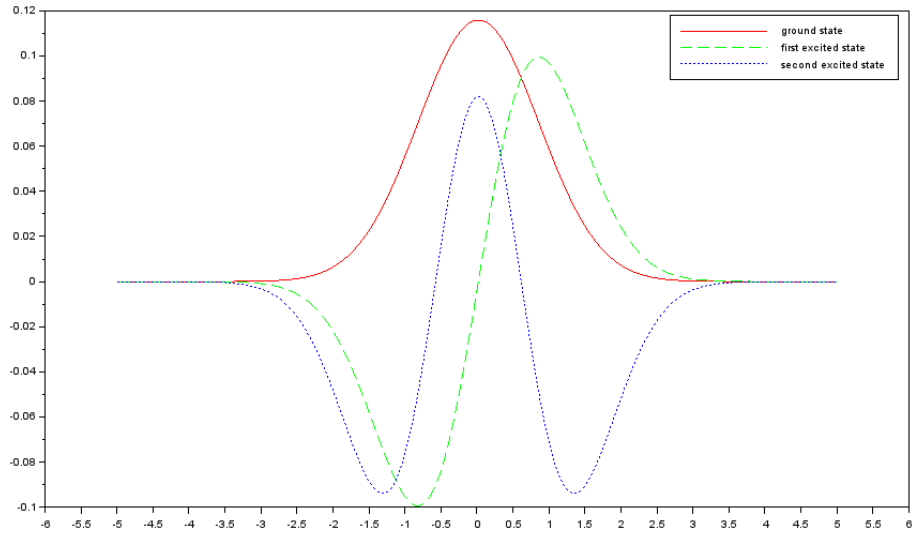
$$-\frac{\hbar^2}{2m}(\frac{\psi(x_{i+1})-2\psi(x_i)+\psi(x_{i-1})}{h^2}) + V(x_i)\psi(x_i) = E\psi(x_i) \tag{11}$$

$$(2+\frac{2mh^2V(x_i)}{\hbar^2})\psi(x_i) - \psi(x_{i+1}) - \psi(x_{i-1}) = \frac{2mh^2E}{\hbar^2}\psi(x_i) \tag{12}$$

Now, the corresponding matrix for this expression would be:

$$\begin{pmatrix} 2+\frac{2mh^2V(x_1)}{\hbar^2} & -1 & 0 & 0 & 0 & 0 & \cdots \\ -1 & 2+\frac{2mh^2V(x_2)}{\hbar^2} & -1 & 0 & 0 & 0 & \cdots \\ 0 & -1 & 2+\frac{2mh^2V(x_3)}{\hbar^2} & -1 & 0 & 0 & \cdots \\ 0 & 0 & -1 & 2+\frac{2mh^2V(x_4)}{\hbar^2} & -1 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} |\Psi\rangle = \frac{2mh^2E}{\hbar^2}|\Psi\rangle \tag{13}$$

Again, the dimensions of this matrix are going to be $(n-1)\times(n-1)$ after applying the normalization conditions. The eigenvalues and eigenvectors of this matrix do infact correspond to the correct solutions. For some reason, unknown as of now, the approximation of $i+\frac{1}{2}$ to $i+1$ did produce the correct results but $i+\frac{1}{2}$ to i just did not. The image of the first three energy state solutions to this problem have been added, and they indeed represent the correct solutions.



3 Conclusion

In this study, the solution of the schrodinger equation for the harmonic oscillator potential was performed numerically in the Scilab language. Two equallty credible substitutions were made for the second derivative. One seemed to produce correct results while the other one did not. The detailed reason for that is still unknown. If the reader identified some mistakes in my procedure, or figured out the reason for the discrepency, he or she is free to contact me through the email provided on the front page. The full code implimentation has been uploaded to the GitHub repository linked https://github.com/dominuszain/TimeIndependentSchrodingerEquation.