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

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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 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 choice of substitution will be done keeping in mind the transformation to a matrix eigenvalue problem. 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 $i+1$ to make the problem solvable by the computation of eigenvalues.

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

$$\frac{d^2}{dx^2}f(x_i) = \frac{f(x_{i+1})-2f(x_i)+f(x_{i-1})}{h^2} \tag{6}$$

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

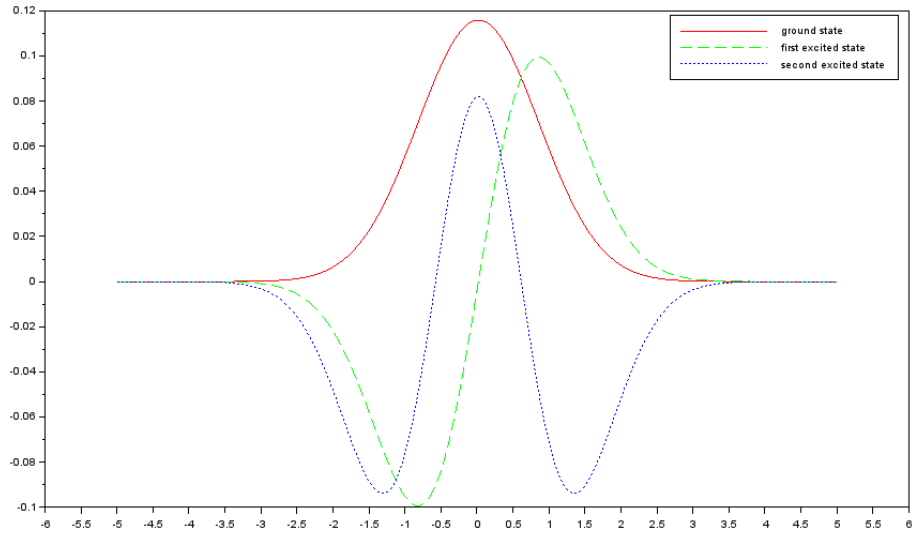
$$-\frac{\hbar^2}{2m}(\frac{\psi(x_{i+1})-2\psi(x_i)+\psi(x_{i-1})}{h^2}) + V(x_i)\psi(x_i) = E\psi(x_i) \tag{7}$$

$$(2+\frac{2mh^2V(x_i)}{\hbar^2})\psi(x_i) - \psi(x_{i+1}) - \psi(x_{i-1}) = \frac{2mh^2E}{\hbar^2}\psi(x_i) \tag{8}$$

Now, the corresponding matrix for this expression would be:

$$\begin{pmatrix} 2+\frac{2mh^2V(x_1)}{\hbar^2} & -1 & 0 & 0 & 0 & \cdots \\ -1 & 2+\frac{2mh^2V(x_2)}{\hbar^2} & -1 & 0 & 0 & \cdots \\ 0 & -1 & 2+\frac{2mh^2V(x_3)}{\hbar^2} & -1 & 0 & \cdots \\ 0 & 0 & -1 & 2+\frac{2mh^2V(x_4)}{\hbar^2} & -1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} |\Psi\rangle = \frac{2mh^2E}{\hbar^2}|\Psi\rangle \tag{9}$$

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 Conclusion

In this study, the solution of the schrodinger equation for the harmonic oscillator potential was performed numerically in the Scilab language. 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.