Numerov's Method

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1 The Physics

1.1 Summary of Problem

We are asked to consider a nucleon trapped in a one-dimensional squared well potential of depth $V_0 = 83MeV$ and $|x| \leq a$ where $a = 2fm$ ($1fm = 10^{-15}m$). We then wish to find the wave function for this particle and the energy of the quantum states it inhabits. We also say for this problem that $\frac{2m}{\hbar^2} = 0.04829MeV^{-1}fm^{-2}$. This project has many similarities to Transcendental Equations, however our goal with this project is to generalize this solution so we can begin considering varying wells of potential.

1.2 Analytical Solution

For our particle, we have the wave function

$$\begin{aligned}\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}\left(E + V_0\right)\Psi = 0 \\ \frac{d^2\Psi}{dx^2} + k^2(x)\Psi = 0\end{aligned} \tag{1}$$

Where $k(x) = \sqrt{\frac{2m}{\hbar^2}(E + V_0)}$ Notice that 1 is of the form of a second order differential equation, missing a first order derivative. This means that we can apply Numerov's Method. For a more in depth analysis on the analytical portion of this problem, refer to Section I of Transcendental Equations. We will delve more deeply into the analytical solution here and how it might be further generalized.

2 Numerical Solution

2.1 Numerov's Method

Numerov's method is used to solve second order differential equations when it lacks a first order term - as we have showed in 1. If we have a differential equation of the form

$$\frac{d^2y}{dx^2} = -g(x)y(x) + s(x) \quad x \in [a, b] \tag{2}$$

Where $g(x)$ and $s(x)$ are continuous from a to b. If we take a look at some step size h, then we can expand $\Psi(x)$ as a Taylor series

$$\begin{aligned}\Psi(x+h) &= \Psi(x) + h\Psi^{'}(x) + \frac{h^2}{2}\Psi^{''}(x) + \frac{h^3}{3!}\Psi^{'''}(x) + ... \\ \Psi(x-h) &= \Psi(x) - h\Psi^{'}(x) + \frac{h^2}{2}\Psi''(x) - \frac{h^3}{3!}\Psi^{'''}(x) + ... \\ \Psi(x+h) + \Psi(x-h) &= 2\Psi(x) + h^2\Psi^{''}(x) + \frac{h^4}{12}\Psi^{iv}(x) + ...\end{aligned} \tag{3}$$

$$\Psi^{''} = \frac{\Psi(x+h) + \Psi(x-h) - 2\Psi(x)}{h^2} - \frac{h^2}{12}\psi^{iv}(x) + O(h^4) \tag{4}$$

Since we end up with a final term of the order of h^4, if we pick a small enough step size, those terms will drop off quickly and can be ignored. Next, we plug this back into the 1 to get

$$\frac{\Psi(x+h)+\Psi(x-h)-2\Psi(x)}{h^2}+k^2\Psi+\frac{h^2}{12}\frac{d^2}{dx^2}\left(k^2\Psi\right)=0 \tag{5}$$

Now, we can take the last term of 5 and expand it out as

$$\frac{h^2}{12}\frac{d^2}{dx^2}(k^2\Psi)=\frac{\left[k^2(x+h)\Psi(x+h)-k^2(x)\Psi(x)\right]+\left[k^2(x-h)\Psi(x-h)-k^2(x)\Psi(x)\right]}{h^2} \tag{6}$$

Which we can then rearrange and collect terms to get

$$\Psi(x+h)=\frac{2\left[1-\frac{5}{12}h^2k^2(x)\right]\Psi(x)-\left[1+\frac{h^2}{12}k^2(x-h)\right]\Psi(x-h)}{\left[1+\frac{h^2}{12}k^2(x+h)\right]} \tag{7}$$

Or rather, simplifying our notation

$$\Psi_{i+1}=\frac{\left[1-\frac{5}{12}h^2k_i^2\right]\Psi_i-\left[1+\frac{h^2}{12}k_{i-1}^2\right]\Psi_{i-1}}{1+\frac{h^2}{12}k_{i+1}^2} \tag{8}$$

Which gives us an equation to find the following value of the Schrodinger equation. This does rely upon

3 Program

4 Analysis