Numerically solving the one-dimensional Schrodinger equation

The Numerov Method

A one-dimensional Schrodinger equation for a particle in a potential can be numerically solved on a grid which discretizes the position variable using a finite difference method. The TISE is

$$\left[T+V\left(x\right)\right]\psi\left(x\right)=E\psi\left(x\right) \tag{1.1}$$

with $T=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$, which we can write as

$$\psi''\left(x\right)=-k^2\left(x\right)\psi\left(x\right) \tag{1.2}$$

where $k^2\left(x\right)=\frac{2m}{\hbar^2}\left[E-V\left(x\right)\right]$.

If we discretize the variable x, choosing a grid spacing dx over which V varies slowly, we can use a three point finite difference to approximate the second derivative:

$$f_i''\approx\frac{1}{\delta x^2}\left(f\left(x_{i+1}\right)-2f\left(x_i\right)+f\left(x_{i-1}\right)\right) \tag{1.3}$$

The discretized Schrodinger equation can then be written in the form

$$\psi\left(x_{i+1}\right)-2\psi\left(x_i\right)+\psi\left(x_{i-1}\right)=-k^2\left(x_i\right)\psi\left(x_i\right) \tag{1.4}$$

Using the equation for $\psi\left(x_{i+1}\right)$, one can iteratively solve for the eigenfunction. In practice you discretize over a range of space such that the highest and lowest values lie in a region where the potential is very high or forbidden. Splitting the space into N points, chose the first two values $\psi\left(x_1\right)=0$ and $\psi\left(x_2\right)$ to be a small positive or negative number, guess E, and propagate iteratively to $\psi\left(x_N\right)$. A comparison of the wavefunctions obtained by propagating from x_1 to x_N with that obtained propagating from x_N to x_1 tells you how good your guess of E was.

The Numerov Method improves on eq. (1.4) by taking account for the fourth derivative of the wavefunction $\Psi^{(4)}$, leading to errors on the order $O\left(\delta x^6\right)$. Equation (1.3) becomes

$$f_i''\approx\frac{1}{\delta x^2}\left(f\left(x_{i+1}\right)-2f\left(x_i\right)+f\left(x_{i-1}\right)\right)-\frac{\delta x^2}{12}f_i^{(4)}. \tag{1.5}$$

By differentiating (1.2) we know $\psi^{(4)}\left(x\right)=-\left(k^2\left(x\right)\psi\left(x\right)\right)''$, and the discretized Schrödinger equation becomes

$$\begin{aligned}\psi''\left(x_i\right)=&\frac{1}{\delta x^2}\left(\psi\left(x_{i+1}\right)-2\psi\left(x_i\right)+\psi\left(x_{i-1}\right)\right)+\\&\frac{1}{12}\left(k^2\left(x_{i+1}\right)\psi\left(x_{i+1}\right)-2k^2\left(x_{i+1}\right)\psi\left(x_i\right)+k^2\left(x_{i+1}\right)\psi\left(x_{i-1}\right)\right)\end{aligned}. \tag{1.6}$$

This equation leads to the iterative solution for the wavefunction

$$\psi\left(x_{i+1}\right)=\left(1-\frac{\delta x^2}{12}k^2\left(x_{i+1}\right)\right)^{-1}\left(\psi\left(x_i\right)\left(2+\frac{10\delta x^2}{12}k^2\left(x_i\right)\right)-\psi\left(x_{i-1}\right)\left(1-\frac{\delta x^2}{12}k^2\left(x_{i-1}\right)\right)\right). \tag{1.7}$$