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

$$[T + V(x)]\psi(x) = E\psi(x)$$  \hspace{1cm} (1.1)

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

$$\psi''(x) = -k^2(x)\psi(x)$$  \hspace{1cm} (1.2)

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

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:

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

The discretized Schrodinger equation can then be written in the form

$$\psi(x_{i+1}) - 2\psi(x_i) + \psi(x_{i-1}) = -k^2(x_i)\psi(x_i)$$  \hspace{1cm} (1.4)

Using the equation for $\psi(x_{i+1})$, 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 $\psi(x_1) = 0$ and $\psi(x_2)$ to be a small positive or negative number, guess $E$, and propagate iteratively to $\psi(x_N)$. 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 $O(\delta x^6)$. Equation (1.3) becomes

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

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

$$\psi''(x_i) = \frac{1}{\delta x^2} \left( \psi(x_{i+1}) - 2\psi(x_i) + \psi(x_{i-1}) + \right.$$

$$\left. \frac{1}{12} \left(k^2(x_i)\psi(x_{i+1}) - 2k^2(x_i)\psi(x_i) + k^2(x_{i-1})\psi(x_{i-1})\right) \right) \hspace{1cm} (1.6)$$

This equation leads to the iterative solution for the wavefunction

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