Honors Project Physics 448 Fall 2011

There is a specialized method, called the Numerov method, for numerically integrating differential equations of the form

$$\psi'' = f(x)\psi$$

The method, which you can read about on Wikipedia, approximately calculates ψ at a set of *N* discrete positions x_i. Specifically it is a formula for ψ_{i+1} in terms of $\psi_i, \psi_{i-1}, f_{i+1}, f_i$, and f_{i-1}. Your job is write a Mathematica program that will find the eigenvalues and eigenfunctions of the Schrodinger equation for a potential *V(x)* that has a characteristic length scale *a*. Here's how to proceed.

First, find *f(x)*, then write it in terms of an appropriately scaled length *s=x/a* and a corresponding scaled energy variable ε, so that $\hbar$ and *m* are eliminated from the equations. Next, rewrite the Numerov formula in the following manner. Consider ψ to be a length *N* vector whose elements are the ψ_i. The Numerov formula can then be rewritten in the form

$$A\psi + BU\psi = \varepsilon B\psi$$

where *A* and *B* are *NxN* matrices and *U* is an *NxN* diagonal matrix. Multiply by B^{-1} to put the Numerov formula in eigenvalue form

$$K\psi + U\psi = \varepsilon\psi$$

In this form, you can numerically find the eigenvalues and eigenvectors of the Schrodinger equation for, in principle, any potential.

As a test case, find the lowest 20 eigenvalues and eigenvectors of the simple harmonic oscillator. Your results should be accurate to better than 0.1% in the energy. You will need to adjust *N* and the distance δs between points to get sufficient accuracy. Calculate the uncertainty product for the 17th eigenvector and compare to theory. When you get this working, show me your program and I will give you a new potential to solve using it.

Write a short paper describing your theory and calculations. The student with the best solution will be invited to be a coauthor on a short paper on this topic to be submitted to the *American Journal of Physics.*

The paper and program are due Dec. 2.