Energy Eigenvalues and Eigenvectors of Schrödinger's Equation

Extra Credit Project

[due by April 30th, 2009]

Schrödinger's equation is fundamental to modern quantum mechanics. It is a second order differential equation, which has analytical solutions in only a few selected cases. Solutions to most situations must be obtained numerically. Schrödinger's equation (time-independent, one-dimensional) for a particle of mass **m** is:

$$\frac{-\hbar^2}{2\,\mathrm{m}}\frac{d^2\Psi}{dx^2}+V(x)\Psi=E\Psi \qquad (14.1)$$

Normally one would take units in which $\hbar^2/m=1$ to simplify the algebra. This equation then becomes:

$$\frac{-1}{2}\frac{d^2\Psi}{dx^2}=[E-V(x)]\Psi \qquad (14.2)$$

This equation is similar to many other second order differential equations, with one interesting twist, the energy, **E**, is also unknown. Consequently, the numerical solution of this equation must determine both Ψ **(x)** and **E**. For many other applications of second-order differential equations, one starts with an initial condition for Ψ **(x)** and for Ψ' **(x)** and propagates forward and/or backward in steps of Δ**x** until a solution is obtained for the range of interest. The initial conditions for wave functions are obtained in a somewhat different fashion.

When the potential is symmetric, one can use the symmetry to an advantage. Namely, the wave functions can be written as purely odd or purely even functions of **x**. An even parity solution requires that **d**Ψ / **dx = 0** at **x = 0**. One is free to choose $\Psi(0)$ **= 1** and be assured that the solution will be a simple multiple of the one we find. One can later use the normalization condition to determine the precise multiplier. For an odd parity solution one must have $\Psi(0)$ **= 0** and **d**$\Psi(0)$ / **dx** $\neq$ **0**. Again one is free to set **d**$\Psi(0)$ / **dx = 1** and rely upon the normalization condition to determine the "magnitude" of the solution.

By exploiting the symmetry, one has determined the initial conditions for this problem. One can proceed as usual to rewrite the second-order ODE as two first-order differential equations and implement the fourth-order Runge-Kutta method. (See the lecture notes on how to implement the Runge-Kutta 4 method)

The procedure for solving Schrödinger's equation would be identical to any other second-order differential equation with known boundary conditions were it not for two related facts: one does not know **E**, and $\Psi(x)$ must vanish as **x** becomes large. If $\Psi(x)$ does not vanish as **x** becomes large then the normalization integral is not finite and one does not have a physical solution. As it turns out this condition is met only for certain precise values of **E**. In this sense the normalization condition required for $\Psi(x)$ and energy quantization are closely related.

The method of solution for Eqn. 14.2 is to pick a values of **E**, propagate the solutions (for a given parity) to large **x** to determine if they match the boundary condition at large **x**. If they do not, adjust the value of **E** and try again. This process can take good advantage of the root finding techniques described early on in the semester. One way is to start with a very low energy and determine the sign of Ψ at large **x** (or the **x** value where Ψ must vanish) and then increment **E** until the sign of Ψ changes. Once two values of **E** have been obtained that give different signs for Ψ at large **x**, then one of the bracketing methods that was used in Project #7 can be applied. Higher energy solutions of the same parity can be found by incrementing your guess for **E** until Ψ **(large)** changes sign again. Such methods are known as shooting and matching methods.

- Develop a C++ class object for a WaveFunctionCalculator (#include RungeKutta.h)

  Template: /export/home/crede/comphy/src/quantumWave.cc

- Numerically solve Schrödinger's wave equation to find the ground state, 1st , and 2nd excited states energies for an infinite square well of width **2L**. In this case the boundary condition at large **x** is that $\Psi(\pm L) = 0$.

  1. Plot your results for the ground state, 1st, 2nd, and 3rd excited states.

  2. Compare the numerical results for the ratio of these energies to the expected result, **~n^2** (actually $\pi^2/8\,n^2$).

- Solve for the wavefunction of a linear potential:

(There are no analytic results with which to compare.) $V(x) = V_o|x|$ Find the ground state, 1st, 2nd, and 3rd excited states wavefunctions and their energies

- Numerically solve Schrödinger's wave equation to find the ground state, 1st, 2nd, and 3rd excited states wavefunctions and their energies for a potential of $\mathbf{V(x) = x^2}$.

- Numerically solve Schrödinger's wave equation to find the ground state, 1st, 2nd, and 3rd excited states wavefunctions and their energies for a potential of $\mathbf{V(x) = x^4}$.

Record your work and report your results on your computational physics website. Create a html page for this exercise. Create a link from your main project web page to this html page. This html page should include the following heading information: exercise title, exercise number, your name, & today's date. The main content of this page should include the following:

- a short description of the exercise
- a table of energy eigenvalues for each potential
- a link to class header and source code files
- images (not links) of your plots for $\Psi(x)$ vs x for the ground state of each potential