Lab 9

Thursday 8 November 2007 - Due: Thursday 15 November

In this lab we will learn how to solve the Schrodinger equation for simple 1D bound state problems.

1 Quantum Harmonic Oscillator

1. Download the code `qm.py` from the course webpage. This code prompts you to guess an allowed energy and with that it computes a trial wavefunction using leapfrog integration. Notice that you type your guess directly into the python interactive window. The program loops for ever until you kill it explicitly.

2. Find the allowed energy which lies in the range $E = 0.0 - 1.0$. To zero in on the allowed energy notice how the trial wavefunction behaves at large x – if for energy $E = E_1$ it diverges to large, positive values at large x while at $E = E_2$ it starts to diverge to large, negative values then the allowed energy lies somewhere in the range $E_1 < E < E_2$. Locate the energy to three decimal places. Show a plot of the allowed state/wavefunction.

3. Find a similar allowed energy in the range $2.0 - 3.0$. You may want to increase the integration region defined by parameter `BOX` from 3.0 to 4.0. This reflects the fact that allowed wavefunctions spread further as the energy increases. Plot the allowed wavefunction again.

4. The initial conditions that have been used allow us to find only wavefunctions that are symmetric about the origin. There exist another set which are *antisymmetric* about the origin. These can be accessed by setting

   ```
   phi[0]=0.0
   p[0]=1.0
   ```

   Change to these initial conditions in the code and search for further allowed energies in the ranges $1.0 - 2.0$ and $3.0 - 4.0$. Plot out also the wavefunctions of these stationary states.

5. Can you guess a simple formula for the energies of these allowed states in terms of the integers $n = 0, 1, 2, \ldots$? How many peaks are seen in the wavefunctions as n increases ?

6. Now locate the code which defines the potential function `V(x)`. Modify the potential from $\frac{1}{2}x^2$ to $\frac{1}{2}\omega^2 x^2$. Set $\omega = 2$ and recompute the energies (you may need to reduce `BOX` by a factor of two or so relative to its value for $\omega = 1$. You may also want to experiment with increasing the number of points used in the integration from `N=10000` to larger values)

7. What is the ratio of the ground state energy (the state with smallest allowed energy) with $\omega = 1$ to that with $\omega = 2$?

2 Quantum box

1. Modify the code to model a quantum well with depth H and width $2a$ with potential function

$$\begin{aligned} V(x) &= 0 \qquad x < -a \\ V(x) &= 0 \qquad x > a \\ V(x) &= -H \qquad -a \leq x \leq a \end{aligned}$$

   Set $a = 1.0$ and $H = 5.0$.

2. Determine the allowed energies and wavefunctions of an electron confined to this quantum well for both even and odd initial conditions.

3. What happens for $E > H$? Do the allowed wavefunctions behave exponetially for large x ?