

### Computer Assignment 3

#### *Eigenstates of General Hamiltonians in 1d*

In this assignment you will calculate energy eigenvalues using a symbolic algebra program, but this time the Hamiltonian matrix is not readily available. You will have to choose a basis set and evaluate the matrix elements by performing the integrals.

The system is a particle of mass  $m=1$  in a potential  $V(x)$  (to be specified below). Thus, the Hamiltonian has the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}).$$

Your goal is to calculate the five lowest energy eigenfunctions and eigenvalues with accuracy of 0.1% in the energies. For convenience I suggest using particle-in-a-box basis functions. You should do this for two potentials, (i)  $V(x) = \frac{1}{2}x^2$  and (ii)  $V(x) = \frac{1}{2}x^4$ . I recommend you write the program with the harmonic potential in mind, in which case you know the answers, so you can check things. Once everything is ok, you could copy the program and replace the potential function.

(a) To get started, you need to choose the size of the box. Estimate the spatial range (i.e., the distance between turning points) of the highest energy eigenfunction you need. You do not need to be accurate here. Since the potential is symmetric, you should choose a box placed symmetrically about the potential minimum with length about 20-30% larger than the estimated range of your eigenfunctions (that's because the wavefunctions extend beyond classical turning points). Next, choose the number  $N$  of basis functions you would like to use. I suggest you start with 5-10 basis functions.

(b) Define the basis functions in your symbolic algebra program using the form obtained in class.

(c) Have your symbolic algebra program calculate the matrix elements of the Hamiltonian. To do this you need to calculate (i) potential integrals and (ii) kinetic energy integrals. You already did this in Computer Assignment 1, so you may copy those operations and paste them in this program.

(d) Now your Hamiltonian matrix is ready, so you may proceed as in the previous assignment. However, you have just obtained the matrix in numerical form, so you should expect to obtain eigenvalues and eigenvectors as numbers. Make sure your eigenvectors are normalized. (If necessary, perform the required operation to normalize them.)

(e) Examine the lowest eigenvalues. Hopefully, they will not look extremely unreasonable. Now you need to vary your parameters until you have converged to the required accuracy. Start by increasing the number of basis functions a little. Are the eigenvalues changing significantly?

Once they stop changing, you know you've got enough basis functions. Increase the box size a bit. Be careful here, you don't want to increase it too much because this means you will not have enough basis functions in the energy range of interest! Redo the calculation with the larger box and again check convergence with respect to basis set size. Repeat these steps until you have converged the lowest five eigenvalues to the specified accuracy. You should compare to the known results for the harmonic potential. How do the results differ in the case of the quartic potential?

(f) Construct the wavefunctions of the five lowest energy states from the basis functions and the calculated eigenvector coefficients. Plot these functions.

Note: It is convenient to work in atomic units. In these units,  $\hbar = 1$ .