Practical work 1: Calculation of energy levels for one-dimensional systems.

1 Introduction.

The aim of this work is to evaluate numerically the energies of bound and resonant states for some simple 1-D problems. To obtain these energies we expand the corresponding eigenfunctions in terms of appropriate basis functions. Using atomic units, the Hamiltonian of the system has the form:

$$H = -\frac{1}{2m}\nabla^2 + V(x) \tag{1}$$

The eigenfunctions of this Hamiltonian, ψ_n, are expanded as linear combinations of the orthonormal basis functions $\{\phi_k\}$:

$$\psi_n(x) = \sum_k c_{kn}\phi_k(x) \tag{2}$$

Using the variational method, the coefficients and the energies are the solutions of the matrix eigenvalue equation:

$$\underline{\boldsymbol{H}}\,\underline{\boldsymbol{c_n}} = E_n\underline{\boldsymbol{c_n}} \tag{3}$$

where the elements of the matrix $\underline{\boldsymbol{H}}$ are:

$$H_{ij} =< \phi_i|H|\phi_j > \tag{4}$$

2 Functions of the 1D square well potential.

We consider the eigenfunctions of the 1D Hamiltonian (1) with

$$\begin{aligned} V(x) &= \infty \quad \text{for } x > L/2 \text{ or } x < -L/2 \\ V(x) &= 0 \quad \text{for } -L/2 < x < L/2 \end{aligned} \tag{5}$$

Work following this scheme:

1. Evaluate analytically the integral $< \phi_1|x|\phi_2 >$
2. We shall also use the integrals $< \phi_i|x^2|\phi_j >$ and $< \phi_i|p^2|\phi_j >$. Check:
   (a) $< \phi_i|x^2|\phi_j >$ vanishes for $i + j$ odd
   (b) $< \phi_i|p^2|\phi_j >$ is a diagonal matrix, where $< \phi_i|p|\phi_j >= \left\langle \phi_i \left| -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} \right| \phi_j \right\rangle$.

3. These integrals have been programmed in the MATLAB routine **kgbox.m**. Check the results running this program by writing in the MATLAB command window:

   [x,x2,p2]=kgbox(N,L)

   with e.g. N=4 (number of basis functions) and L=1 (box length).

4. Write the following commands:

   [x,x2,p2]=kgbox(4,1);
   xsq= x*x;
   xsq(2,4)-x2(2,4)
   [x,x2,p2]=kgbox(50,1);
   xsq= x*x;
   xsq(2,4)-x2(2,4)

   Discuss the result.

3 Energies of bound states.

We can use the matrix elements calculated in the previous section to obtain the energies of some 1D systems. We consider first the harmonic oscillator:

$$H = \frac{p^2}{2m} + m\omega^2 \frac{x^2}{2} \tag{6}$$

The routine **harmonic(mass,omega)** calculates the eigenvalues of the harmonic Hamiltonian; this programm carries out the following operations:

1. It creates a grid of values of the box length L.
2. It calculates the matrix elements of H using the integrals evaluated by **kgbox**.
3. It diagonalizes the matrix $\underline{\boldsymbol{H}}$ using the MATLAB command **eig**
4. It plots the energies as functions of L and compares them with the exact values.

Run the program with ω=0.3 and $m = 1$. Press *intro* to see the comparison with the analytical values. Explain the meaning of the figure obtained. Which are the values of the energies in the limit of small L?

The second example is the Morse potential:

$$V(x) = D\left(1 - \mathrm{e}^{-\beta x}\right)^2 \tag{7}$$

Plot the potential for $D = 10$, $\beta = 0.3$:

ezplot('10*(1-exp(-0.3*x))^2',[-3,10])

The program **morsebox(mass,D, beta)** evaluates the eigenvalues of this problem using a similar method to that applied for the harmonic oscillator and compares the results with the analytical values. Write:

morsebox (1,10.0,0.3)

Edit the file **morsebox.m** and change the value of N (the number of basis functions) to $N = 25$. Run the modified program and discuss the results.

4 Energies of resonant states.

In this example we consider the potential:

$$V(x) = \left(\frac{x^2}{2} - J\right) \exp\left(-\lambda x^2\right) + J \tag{8}$$

Plot this potential for $\lambda = 0.1$, $J = 0.8$:

```
lambda=0.1;
J=0.8;
x=-10:0.1:10; pot= (x.^2/2-J).*exp(-lambda*x.^2)+J;
plot (x,pot);
```

The eigenvalues of this potential are calculated in the program **resonances.m**. Write ($m = 1$,$\lambda = 0.1$, $J = 0.8$)

resonances(1, 0.1, 0.8)

We obtain an energy diagram where the eigenvalues of this potential are plotted as functions of the length of the potential box employed to build up the basis set. We can note:

1. There is a bound state of this potential. Find its energy.

2. There are two states whose energies are independent of the size of the box. They are resonant states, whose wavefunctions are localized inside the potential well. The plot is an example of the stabilization method, where the energies of the resonant states are those which do not change when the basis set is modified.

To further illustrate the method, the program plots the potential and the energy levels for $L = 15$ and $L = 30$a.u.. The corresponding figures are obtained by pressing *intro*. Repeat the calculation for $\lambda = 0.1$, $J = 0.3$

The program also allows us to plot the eigenfunctions for $L = 30$a.u.. For example,

resonances(1, 0.1,0.8, 1, 5,8,12)

plots the eigenfunctions ψ_j with $j = 1$, 5, 8 and 12. Discuss the figure obtained.

5 References.

H. J. Korsch and M. Glück, Eur. J. Phys. **23** (2002) 413-26