PH3105 Problem Set 8

One of the methods for solving an eigenvalue equation is the so called shooting method. Let me illustrate this with an example that tries to find the first few eigenvalues for the one dimensional Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \tag{0.1}$$

We will begin with the harmonic potential $V(x) = \frac{1}{2}m\omega^2x^2$. Let us first rewrite the equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi \tag{0.2}$$

in a dimensionless form more suitable for numerical computation. A simple rescaling of the variable x leads to the equation

$$\frac{d^2\psi}{dx^2} + \left(\lambda - x^2\right)\psi = 0 \tag{0.3}$$

where the eigenvalue λ is related to the energy by $\lambda = \frac{2E}{\hbar\omega}$. Note that the value of λ will be quantized to the familiar values of $2n+1,\ n \in \mathbb{Z}$ once we impose the boundary conditions $\psi \to 0$ as $x \to \pm\infty$. We can't do a numerical integration from $x \to -\infty$ all the way to $x \to +\infty$. So, we will stick to slightly different boundary conditions : $\psi \to 0$ as $x \to \pm L$, where L is sufficiently large. Indeed if we chose L so large that the energy eigenfunctions for the exact problem are very small for $|x| > L$, then the results we will get for λ will come close to the exact ones. In the following we will take $L = 5$ - as we will see, this gives us quite accurate results for the quite a few of the lower eigenvalues.

In order to solve this we start by discretizing (0.3) by using the approximation

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

to get (using the familiar notation $\psi_n = \psi(x_n)\,,\ x_n = -L + nh$

$$\frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{h^2} + \left(\lambda - x_n^2\right)\psi_n = 0$$

which can be rewritten to yield

$$\psi_{n+1} = \left[2 - h^2\left(\lambda - x_n^2\right)\right]\psi_n - \psi_{n-1} \tag{0.4}$$

This allows us to calculate ψ_{n+1} from any two preceding values of ψ.

To start the solution then, we will need the values of ψ_0 and and ψ_1 - all subsequent values will follow (for a particular value of λ). In this case, ψ_0 is already known $\psi_0 \equiv \psi(-L) = 0$. What about ψ_1? The answer is that it (almost) does not matter. Since (0.3) is linear, if $\psi(x)$ is a solution, so is any multiple. We will take $\psi_1 = 1.0$ (Can you figure out why I said (almost) a while ago?). Of course, if you used any value for λ, you will not get $\psi(+L) = 0$. The correct values of λ are the ones that make $\psi(+L)$ vanish. It is as if you were aiming at the target (in this case, getting $\psi(L) = 0$) and adjusting your aim (the value of λ) until you get as close as you need - hence the name "shooting method".

Let us define a python function called psiAtL() which does just what its name suggests, starting from $\psi_0 = 0$ and $\psi_1 = 1$, it calculates the value of $\psi(+L)$

```
def psiAtL(lam):
    p0, p1 = 0.0,1.0
    x = -L+h
    while x<=+L:
         p0,p1 = p1,(2-h**2*(lam-x**2))p1-p0
         x += h
    return p1
```

To find the eigenvalues - all we have to do next is solve for the roots of this function using, say, the bisection method. One word of warning - this is a very steep function of λ - so your stopping criterion should be making the bracketing interval sufficiently small - as opposed to trying to make $|\psi(+L)|$ very small.

Q 1) Write a program that uses the shooting method to determine the lowest five eigenvalues of (0.3)

Q 2) Modify the program slightly to find the eigenvalues of an anharmonic oscillator with potential

$$V(x) = x^2 + \alpha x^4$$

Use your program to plot the variation of the energy eigenvalue versus the parameter $\alpha$for at least the three lowest eigenvalues (α ranging from 0 to 1).

Q 3) Find the lowest three eigenvalues for the potential

$$V(x) = \begin{cases} \infty & x \leq 0 \\ x, & x > 0 \end{cases}$$

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While the method outlined above works to some extent, the integration routine outlined in (0.4) is of limited accuracy. We will now study a more accurate algorithm called the Numerov algorithm which takes advantage of the particular structure of the Schrödinger equation (0.1) (it is linear and there is no term involving the first derivative). We first write the equation in a slightly more convenient form

$$\psi''(x) + k^2(x)\,\psi(x) = 0 \tag{0.5}$$

where $k^2(x) = \dfrac{2m}{\hbar^2}(E - V(x))$.
From the Taylor series one can easily show that

$$\psi''(x) = \frac{\psi(x+h) - 2\psi(x) + \psi(x-h)}{h^2} - \frac{h^2}{12}\psi^{(4)}(x) + \mathcal{O}\left(h^4\right)$$

We can differentiate (0.5) twice to obtain

$$\psi^{(4)}(x) = -\left[k^2(x)\,\psi(x)\right]''$$

so that we can write (0.5) in the form

$$\psi_{n+1} + \psi_{n-1} - 2\psi_n + h^2 k^2(x_n)\,\psi_n + \frac{h^4}{12}\left[k^2(x)\,\psi(x)\right]'' + \mathcal{O}\left(h^6\right) = 0$$

Finally we approximate $\left[k^2(x)\,\psi(x)\right]''$ by

$$\frac{k^2(x_{n+1})\,\psi_{n+1} + k^2(x_{n-1})\,\psi_{n-1} - 2k^2(x_n)\,\psi_n}{h^2}$$

and rearrange to get an estimate for ψ_{n+1} which is accurate up to $\mathcal{O}\left(h^5\right)$ locally. This is the **Numerov algorithm**.

4) Use the Numerov algorithm to solve for the lowest four eigenvalues of the harmonic oscillator.

Q 5) The Morse potential

$$V(x) = D\left(e^{-2a(x-x_0)} - e^{-a(x-x_0)}\right)$$

where D and a are constants, is one of the very few potentials for which the Schrödinger equation can be solved analytically. Show that for an appropriate change of variables, the equation can be written in the form (0.5) with

$$k^2(x) = \lambda - \mu^2\left(e^{-2x} - e^{-x}\right)$$

Use the shooting method with the Numerov algorithm to find the first eight eigenvalues of the Morse potential.

Q 6) We can of course write (0.5) in the form

$$\frac{d\psi}{dx} = \phi$$
$$\frac{d\phi}{dx} = -k^2(x)\,\phi$$

of coupled first order differential equations. We can solve these using RK4 and then apply the shooting method. Solve Q5 using this method.