Computational Physics
Topic-III
Boundary value problem

In many physical problems we encounter ordinary differential equations. The solution of an ordinary differential equation requires auxiliary conditions. For an *n*th-order equation, *n* conditions are required. If all the conditions are specified at the same value of the independent variable, we have an *initial-value* problem. Simple harmonic motion is one such example. If the conditions are known at different values of the independent variable, usually at the extreme points or boundaries of a system, we have a *boundary-value* problem. Stationary wave in string, 1 dimensional time independent Schrodinger's equation for a particle in a rigid box are examples of boundary value problems.

A second order differential equation as a boundary value problem is exemplified by the equation

$y'' + \lambda y = 0$ …(1)

Where, the boundary condition is given as $y(a) = y_a$ and $y(b) = y_b$ and we need to solve the differential equation in the region $[a, b]$ of the independent variable. The solution will exist for some special values of λ known as the eigen values. Hence the above problem is also known as an eigen value problem.

Numerical method: The above problem is solved by adopting the same numerical method used for solving initial value problems with different guess values for the eigen value λ and with the initial condition $y(a) = y_a$. This will generate a set of values $y_b(\lambda)$ for $y(b)$ as a function of λ. In general this value will not match with the boundary condition $y(b) = y_b$. For correct choice of λ, the boundary condition should be satisfied and hence, solving the eigen-value problem turns out to be a problem of finding the root of the algebraic equation

$y_b(\lambda) - y_b = 0$ …(2).

Example1: Let us illustrate the method with the specific example of a quantum mechanical particle in a rigid one dimensional box shown in figure 1.

The problem is

$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0$ …(3)

with $V(x) = 0; 0 < x < L$
$= \infty; otherwise$

Hence, within the box, the differential equation becomes

$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$ with the boundary condition

$\psi(0) = \psi(L) = 0.$ …(4)

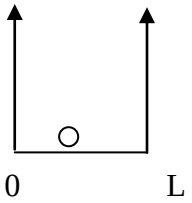

Figure 1

This problem can be solved in three major steps.

Step 1: Treat the problem as an initial value problem (take $(0) = 0$) and adopt Euler method (or any other method for solving ODE) to generate values of $\psi(L)$ for different values of E.

Step 2: Solve for E such that $\psi(L) = 0$. These are the correct eigen values.

Step3: Calculate $\psi(x)$with correct eigen values.

For step 1: Make two initial guesses for E, say E_1 and E_2. Take $\psi(0) = 0$ and assume $\psi'(0) = 1.0$ arbitrarily. Take the values of the constants $(m, \hbar)$ in natural unit for convenience in computation. Compute $\psi_{E_1}(L)$and $\psi_{E_2}(L)$ as shown in the figure 2.

For Step 2: Adopt a root finding routine (namely Secant Method) to solve for $\psi_E(L) = 0$. The following iterative formula generates better guess for the energy eigen value using Secant method (illustrated in figure 3).

$$E_{i+2} = \frac{\psi_{E_i}(L)E_{i+1} - \psi_{E_{i+1}}(L)E_i}{\psi_{E_i}(L) - \psi_{E_{i+1}}(L)} \quad \ldots(5)$$

Continue this process until $|E_{i+2} - E_{i+1}| \leq \epsilon$ (a predefined small number that sets the accuracy). At the end of this process the solution converges to a correct eigenvalue.

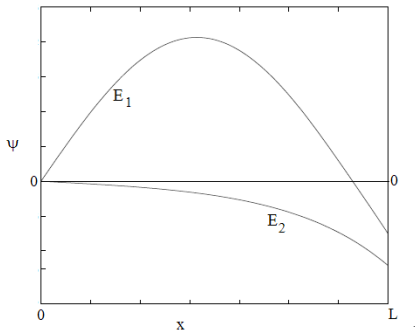

Figure 2

For step 3: Use the same routine of initial value problem for generating $\psi(x)$ in the region $0 \leq x \leq L$ with correct E value but arbitrary value of $\psi'(0) = 1$. This arbitrariness can be removed by normalizing the wave function $\psi(x)$ by multiplying it with the normalization factor defined as $A = \frac{1}{\sqrt{\int_0^L |\psi(x)|^2 dx}}$ where the integration can be evaluated numerically by adopting simple routines like trapezoidal rule.

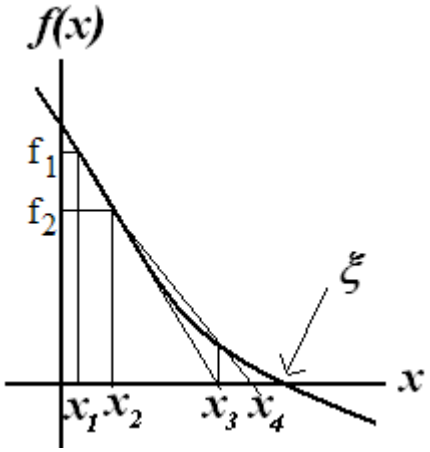

Figure 3

Example 2: Quantum mechanical harmonic oscillator

In this case the problem is defined as

$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0$ with $V(x) = \frac{1}{2}kx^2$. …(6)

Hence the boundary condition becomes $\psi(\pm\infty) = 0$.

This problem is a bit different from the previous one because the wave function does not vanish at finite distance. But numerically this does not make much difference because we can choose a large length $\pm L$ to replace $\pm\infty$. The basic routine remains the same. i.e we shall start from one side and try to mathe the boundary value at the other side. But with a finite potential in the region and with an incorrect value of E (which is guess value and in general incorrect) the value of wave function diverges rapidly. Hence, we modify our strategy accordingly. We shall choose an arbitrary point (may be the classical turning point x_c) within the region $-L \leq x \leq L$. We shall start from both left and right sides with the initial values $\psi_l(-L) = 0$ and $\psi_r(L) = 0$ respectively and calculate $\psi_l(x_c)$ as well as $\psi_r(x_c)$. For incorrect E value these two values will not match as shown in the figure 4(a). But we know that the wave function must be continuous in the region. This condition can be satisfied by multiplying the wave functions by suitable scale factor. For example if we define the scale factor as $s = \frac{\psi_l(x_c)}{\psi_r(x_c)}$ and multiply it with $\psi_r(x_c)$ we

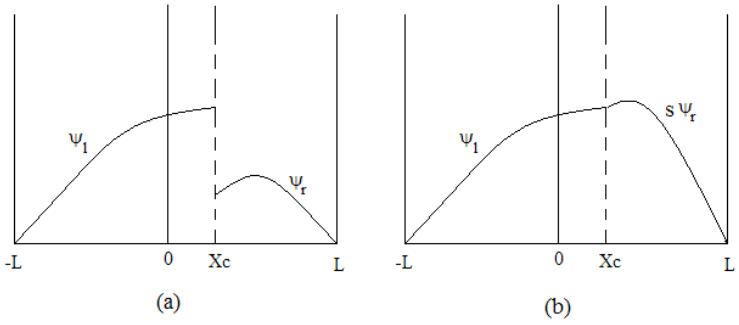

Figure 4:

shall get the continuity of the wave function as shown in figure 4(b). But again the wave function will not be smooth at $x = x_c$which violates the condition for $\psi(x)$ to be an acceptable wave function. To be a well behaved function in the region, the wave function should be smooth everywhere in the region. Hence the first derivative of ψ should be continuous at $x = x_c$.Mathematically, for the scaled wave function, this condition reads like,

$$\frac{\psi_l(x_c + h) - \psi_l(x_c)}{h} = \frac{s\psi_r(x_c + h) - s\psi_r(x_c)}{h}$$

$$=> \psi_l(x_c + h) - s\psi_r(x_c + h) = 0 \quad \ldots \qquad (6)$$

If we define $\Delta\psi_{x_c}(E) = \psi_l(x_c + h) - s\psi_r(x_c + h)$, then the problem of finding eigenvalue becomes a problem of finding the roots of the equation

$\Delta\psi_{x_c}(E) = 0$ …(7)

Now one can use the steps described above for particle in a box problem.

Three point formula for solving ODE.

The differential equation can be expressed as $\psi'' + w(x)\psi(x) = 0$.
Where, $w(x) = \frac{2m}{\hbar^2}[E - V(x)]\psi(x)$.
Expanding in Taylor series we get

$$\psi(x+h) = \psi(x) + h\psi'(x) + \frac{h^2}{2}\psi''(x) + \frac{h^3}{6}\psi'''(x) + \frac{h^4}{24}\psi^{iv}(x) + \cdots \quad (8a)$$

and $\psi(x-h) = \psi(x) - h\psi'(x) + \frac{h^2}{2}\psi''(x) - \frac{h^3}{6}\psi'''(x) + \frac{h^4}{24}\psi^{iv}(x) + \cdots$ (8b)
adding them up, we get,

$$\psi(x+h) + \psi(x-h) = 2\psi(x) + h^2\psi''(x) + O(h^4) + \cdots \quad (9)$$

Hence, neglecting the higher order terms we get the three point formula as

$$\psi''(x) = \frac{\psi(x+h)+\psi(x-h)-2\psi(x)}{h^2} + O(h^2) \quad \ldots(10)$$

This formula can be used to solve for Schrodinger equation with initial value known like an iterative formula as

$$\psi_{i+2} = 2\psi_{i+1} - \psi_i - h^2 w_{i+1}\psi_{i+1} \quad \ldots(12)$$

Fox-Goodwin-Numerov Formula:
The above three point formula leads to an error $O(h^2)$. Now we will see how this error can be reduced by using an improved formula known as *Fox-Goodwin-Numerov Formula*. To obtain this formula we use the same Taylor expansion but with two more terms as shown below.

$$\psi(x+h) = \psi(x) + h\psi'(x) + \frac{h^2}{2}\psi''(x) + \frac{h^3}{6}\psi'''(x) + \frac{h^4}{24}\psi^{iv}(x) + \frac{h^5}{120}\psi^{v}(x) + \frac{h^6}{740}\psi^{vi}(x) \ldots (13a)$$

and $\psi(x-h) = \psi(x) - h\psi'(x) + \frac{h^2}{2}\psi''(x) - \frac{h^3}{6}\psi'''(x) + \frac{h^4}{24}\psi^{iv}(x) - \frac{h^5}{120}\psi^{v}(x) + \frac{h^6}{740}\psi^{vi}(x) \ldots (13b)$
Adding them up we get,

$$\psi(x+h) + \psi(x-h) = 2\psi(x) + h^2\left(1 + \frac{h^2}{12}\frac{d^2}{dx^2}\right)\psi''(x) + O(h^6) + \cdots \quad (14)$$

Let's now apply the operator $1 + \frac{h^2}{12}\frac{d^2}{dx^2}$ on the Schrodinger equation $\psi'' + w(x)\psi(x) = 0$ which gives

$$\left(1 + \frac{h^2}{12}\frac{d^2}{dx^2}\right)\psi'' + w(x)\psi(x) + \frac{h^2}{12}\frac{d^2}{dx^2}\left(w(x)\psi(x)\right) = 0 \ldots(15)$$

Using (14) in (15) and neglecting error $O(h^4)$ we obtain

$$\frac{\psi(x+h)+\psi(x-h)-2\psi(x)}{h^2} + w(x)\psi(x) + \frac{h^2}{12}\frac{d^2}{dx^2}\left(w(x)\psi(x)\right) = 0 \ldots(16)$$

Applying standard three point formula for the 3rd term in (16) we get

$$\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} + w(x)\psi(x) + \frac{h^2}{12}\frac{\left(w(x+h)\psi(x+h) + w(x-h)\psi(x-h) - 2w(x)\psi(x)\right)}{h^2} = 0$$

On manipulation one gets,

$$\psi(x+h)\left(1+\frac{h^2}{12}w(x+h)\right)+\psi(x)\left(\frac{h^2}{12}10w(x)-2\right)+\psi(x-h)\left(1+\frac{h^2}{12}w(x-h)\right)=0$$

On further simplification,

$$\psi(x+h)=\frac{2\psi(x)-\psi(x-h)-\frac{h^2}{12}\left(10w(x)\psi(x)-w(x-h)\psi(x-h)\right)}{1+\frac{h^2}{12}w(x+h)}$$

This can be expressed as a modified three point formula as following,

$$\psi_{i+2}=\frac{2\psi_{i+1}-\psi_i-\frac{h^2}{12}(10w_{i+1}\psi_{i+1}-w_i\psi_i)}{1+\frac{h^2}{12}w_{i+2}} \qquad \ldots(17)$$

Problem set on ODE (boundary value problem):

a) Obtain a three point formula for solving 2nd order ordinary differential equation.
b) A quantum mechanical particle is free to move inside a 1D box of length L with perfectly rigid walls.
   i) Write the algorithm and flowchart for obtaining numerically the energy eigen values and the corresponding normalized eigen functions.
   ii) Convert your flowchart into a FORTRAN program to get a list of eigen values and plot of eigen states
   iii) How can you find the index of the state from the wave function?

c) Suitably modify your three point formula to obtain Fox-Goodwin-Numerov formula for solving a 2nd order differential equation.
d) Write the algorithm and flowchart for solving Schrodinger's equation for a quantum mechanical harmonic oscillator using the above formula.
e) Implement your algorithm using FORTRAN to get the first five eigen values and eigen functions for the above system
f) Incorporate quartic anharmonic term (βx^4) in the potential and study the shift in 1st three eigen values as function of β . Compare your results with the analytical results obtained from time independent perturbation theory for the ground state.
g) Incorporate sextic anharmonic term (γx^6) in the potential and study the shift in 1st three eigen values as function of β . Compare your results with the analytical results obtained from time independent perturbation theory for the ground state.
h) Suitably modify your program to solve the problem of a quantum mechanical particle in a half harmonic potential. Can you predict the eigen values and eigen functions without calculations?