Chapter 4

Boundary Value and Eigenvalue Problems

Solve second order linear differential equation

$$\frac{d^2y(x)}{dx^2} + k^2(x)y(x) = S(x) \tag{4.1}$$

for function $y(x)$. When the source term $S(x)$ is not zero, then this becomes boundary value problem with boundary condition of $y(x_0) = y_0$ and $y(x_N) = y_N$ or as an initial value problem with intitial condition of $y(x_0) = y_0$ and $y'(x_0) = y'_0$ or equivalently $y(x_0) = y_0$ and $y(x_1) = y_1$. If the source term is zero then this becomes eigenvalue problem with boundary condition.

Wave equation for normal mode in 1-d;

$$\frac{d^2\psi(x)}{d^2x} = -k^2(x)\psi(x). \tag{4.2}$$

Poisson equation for electric potential;

$$\nabla^2\phi(\vec{r}) \;\; = \;\; -\frac{1}{\epsilon_0}\rho(\vec{r}). \tag{4.3}$$

Time independent Schrödinger equation;

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) \;\; = \;\; E\psi(\vec{r}). \tag{4.4}$$

In Cartesian 1-d, $\nabla^2 = \frac{d^2}{dx^2}$. In spherical coordinate system,

$$\begin{aligned}\nabla^2 &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} \\ &= \frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{r^2}\frac{L^2}{\hbar^2}. \qquad (4.5)\end{aligned}$$

For spherically symmetric system, i.e., for $\rho(\vec{r}) = \rho(r)$ or $V(\vec{r}) = V(r)$, the variables r, θ, and φ are separable

$$\psi(r,\theta,\varphi) = \frac{R(r)}{r}Y_{lm}(\theta,\varphi) \qquad (4.6)$$

with spherical harmonic Y_{lm}. Then the equation for radial function R becomes

$$\frac{d^2R(r)}{dr^2} + \frac{2m}{\hbar^2}\left[E - V(r) - \frac{l(l+1)\hbar^2}{2mr^2}\right]R(r) = -\frac{1}{\epsilon_0}r\rho(r) \qquad (4.7)$$

where the source term $\rho(r) = 0$ for the time independent Schrödinger equation and $E = 0$ and $V(r) = 0$ for the Poisson equation.

4.1 Numerov Algorithm

When the source $S(x)$ is not zero, the inhomogeneous linear differential equation Eq.(4.1) with boundary condition determines the response $y(x)$ to the source $S(x)$. From Eq.(2.8), for Eq.(4.1),

$$\begin{aligned}y_{n+1} - 2y_n + y_{n-1} &= h^2 y_n'' + \frac{h^4}{12}y_n'''' + O(h^6) \\ &= h^2(S - k^2 y)_n + \frac{h^4}{12}(S - k^2 y)_n'' + O(h^6). \qquad (4.8)\end{aligned}$$

Using Eq.(2.13) for $y'''' = (S - k^2 y)''$,

$$\begin{aligned}\left(1 + \frac{h^2}{12}k_{n+1}^2\right)y_{n+1} &- 2\left(1 - 5\frac{h^2}{12}k_n^2\right)y_n + \left(1 + \frac{h^2}{12}k_{n-1}^2\right)y_{n-1} \\ &= \frac{h^2}{12}\left(S_{n+1} + 10S_n + S_{n-1}\right) + O(h^6). \qquad (4.9)\end{aligned}$$

This recursion relation can be used as an initial value problem. Start with y_0 and y_1 or y_N and y_{N-1}. The response $y(x)$ to the source $S(x)$ can also be found using Predictor-Corrector Algorithm with boundary condition of $y(x_0) = y_0$ and $y(x_N) = y_N$ as discussed in Sect.3.3.

Since Eq.(4.1) is a linear differential equation, a large error at end points could occur even if we start with a small error at initial points. For an inhomogeneous linear differential equation the general solution is a sum of a particular solution of the inhomogeneous equation and a general solution of homogeneous differential equation. As a simple example,

$$\frac{d^2\phi(x)}{dx^2} = e^{-x} \tag{4.10}$$

has solution $\phi(x) = e^{-x}$ with boundary condition $\phi(0) = 1$. The homogeneous equation $d^2\phi(x)/dx^2 = 0$ has a general solution of $\phi(x) = a + bx$ with arbitrary constants a and b. Thus the general solution of Eq.(4.10) is

$$\phi(x) = e^{-x} + a + bx. \tag{4.11}$$

Even if there is only a very small error in initial value y_0 and y_1, the error becomes larger and larger as $a + bx$ form in the recursive steps of Numerov method. However since we know the form of the error occurring due to the solution of homogeneous equation, we can compensate by hand after recursive calculation to remove this type of error. If we use predictor-corrector method with proper boundary condition then this problem does not occur. Another way of avoiding this kind of error is using Green function satisfying boundary condition at both side.

4.2 Green's Function Solution; Boundary Condition

Gauss theorem;

$$\int_V \vec{\nabla} \cdot \vec{A} dV \;=\; \oint_S \vec{A} \cdot d\vec{S}. \tag{4.12}$$

Green's theorem, with $\vec{A} = \phi\nabla\psi$ and $\vec{B} = \psi\nabla\phi$,

$$\int_V \vec{\nabla} \cdot \left(\vec{A} - \vec{B}\right) dV \;=\; \int_V \left[\phi\nabla^2\psi - \psi\nabla^2\phi\right] dV \;=\; \oint_S \left[\phi\vec{\nabla}\psi - \psi\vec{\nabla}\phi\right] \cdot d\vec{S}.$$

For a linear differential equation,

$$\left[\nabla^2 + k^2(\vec{r})\right]\Psi(\vec{r}) = S(\vec{r}), \tag{4.13}$$

the corresponding Green function;

$$\left[\nabla^2 + k^2(\vec{r})\right]G(\vec{r},\vec{r}') = -4\pi\delta(\vec{r}-\vec{r}'). \tag{4.14}$$

Then

$$\begin{aligned}\Psi(\vec{r}) &= -\frac{1}{4\pi}\int G(\vec{r},\vec{r}')S(\vec{r}')dV \\ &+\frac{1}{4\pi}\oint_S \left[G(\vec{r},\vec{r}')\vec{\nabla}'\Psi(\vec{r}') - \Psi(\vec{r}')\vec{\nabla}'G(\vec{r},\vec{r}')\right]\cdot d\vec{S}\end{aligned} \tag{4.15}$$

with Green's function satisfying a proper boundary condition.

In 1-d, the solution $\phi(x)$ of

$$\left[\frac{d^2}{dx^2} + k(x)\right]\phi(x) = S(x) \tag{4.16}$$

with boundary condition of $\phi(x = a) = 0$ and $\phi(x = b) = 0$ for $a \le x \le b$,

$$\phi(x) = \int_a^b G(x,x')S(x')dx', \tag{4.17}$$

where the Green's function $G(x, x')$ satisfies

$$\left[\frac{d^2}{dx^2} + k(x)\right]G(x,x') = \delta(x-x') \tag{4.18}$$

with proper boundary condition, i.e, $G(x, x') = 0$ when either of x or x' is at the bondary point a or b for this case. Integrating this

$$\left.\frac{dG}{dx}\right|_{x=x'+\epsilon} - \left.\frac{dG}{dx}\right|_{x=x'-\epsilon} = 1. \tag{4.19}$$

Using the homogeneous solution $\phi_<$ and $\phi_>$ of the linear differential equation without the source term with proper boundary condition at $x = a$ and $x = b$, i.e., $\phi_<(x = a) = 0$ and $\phi_>(x = b) = 0$, the green function satisfying boundary condition of ϕ is

$$G(x,x') = \phi_<(x_<)\phi_>(x_>) \tag{4.20}$$

with $x_<$ and $x_>$ are the smaller one and larger one of x and x'. Thus

$$\phi(x) \;=\; \phi_>(x)\int_a^x \phi_<(x')S(x')dx' + \phi_<(x)\int_x^b \phi_>(x')S(x')dx'. \tag{4.21}$$

As an example, the radial equation of Poisson equation

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right]\phi(r) \;=\; S(r) \tag{4.22}$$

for $0 \le r < \infty$ has

$$\phi_<(x) = r^{l+1} \quad ; \quad \phi_>(x) = -\frac{1}{2l+1}r^{-l}. \tag{4.23}$$

4.3 Eigenvalue Problem

Homogeneous linear differential equation without source term $S(x)$,

$$\left[\frac{d^2}{dx^2} + k^2(x)\right]\psi_n(x) \;=\; \lambda_n\psi_n(x) \tag{4.24}$$

in the range of $a \le x \le b$. The solution $\psi_n(x)$ can have an arbitrary overall scale thus have a normalization condition. Boundary condition at both end points $\psi(x_a) = \psi_a$ and $\psi(x_b) = \psi_b$ can be satisfied only for special values of λ_n. Such a value of λ_n is called eigenvalue and the corresponding $\psi_n(x)$ is the eigenfunction.

To solve eigenvalue problem use shooting method. Since $\psi_n(x)$ can have an arbitrary overall size, the numerical integral can be started with $\psi_n(a) = \psi_a$ and $\psi_n'(a) = \psi_a'$ with arbitrary value of ψ_a'. If it does not satisfy the boundary condition then do the same thing with a new trial value for λ_n. Repeat this process until the boundary condition is satisfied within allowed error. In choosing a new value of λ_n use the method of finding roots in Sect. 2.5.

If $\psi(x)$ goes to zero exponentially as approaching to the boundaries, then the error coming from the numerical integral is too large to satisfy boundary condition. For such a case, integrate in from both end point with boundary condition and match smoothly the integrated wave function $\psi_<(x)$ and $\psi_>(x)$ at a matching point x_m where ψ is not too small.

$$\psi_<(x_m) = \psi_>(x_m) \quad ; \quad \frac{d\psi_<(x_m)}{dx} = \frac{d\psi_>(x_m)}{dx}. \tag{4.25}$$

Since the normalization condition, the matching condition can be reduced to

$$\frac{\psi_<(x_m - h)}{\psi_<(x_m)} - \frac{\psi_>(x_m - h)}{\psi_>(x_m)} = 0. \tag{4.26}$$