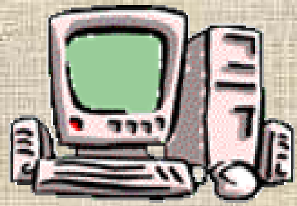

COMPUTATION PHYSICS

PHYS 6312

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CHAPTER 5

Boundary Value Problem And Eigen Value problem

- Most of the important different equations in physics is in the form of 2nd order equation:

$$\frac{d^2 y}{d^2 x} + K^2(x)\, y = S(x)$$

- S(x) is inhomogeneous driving term
- K^2 real function

Poisson's Equation is:

$$\nabla^2 \varphi = -4\pi\rho$$

- For spherical symmetric φ , ρ potential and charge density,

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\Phi}{dr}\right) = -4\pi\rho$$

$$\Phi(r) = r^{-1}\phi(r)$$

$$\frac{d^2\phi}{dr^2} = -4\pi r\rho$$

- $K^2=0$, $S=4\pi\rho r$

•In Q.M., particle with mass m move in a central potential,

- $\psi(r) = r^{-1} R(r)\, Y_{lm} (r)$,
- The radial wave function r satisfies ,
- $d^2R/dr^2 \; + \; K^2 (r) R = 0$
- $K^2 (r) = 2m/h^2 (E – L(L+1)h^2/2mr \;\; -V(r))$

•5.1 Numerov Algorithm:

- $d^2y/dx^2 = (-K^2(x)\, y + S(x))$ (1)
- From the definition of f ``,
- $f`` = (f_1 - 2f_0 + f_{-1})/h^2$
- $y_n`` = (y_{n+1} - 2\, y_n + y_{n-1})/h^2$
- $= y_n`` + h^2/12\, y_n```` + O(h^4)$ (2)

- From the differential equation itself:
- $Y_n```` = d^2/dx^2 (-k^2\, y + S)$
- $= -((k^2y)_{n+1} - 2(k^2y)_n + (k^2y)_{n-1})/h^2$
- $+ (S_{n+1} - 2\, S_n + S_{n-1})/h^2 + O(h^2)$

•Substitute into equation (2) and rearrange,

- $(1+h^2/12 \ K^2_{n+1}) \, y_{n+1}$
- $- 2 (1 - 5h^2/12 \ k_n) \, y_n$
- $+ (1+h^2/12 \, k^2_{n-1}) \, y_{n-1}$
- $= h^2/12 (S_{n+1} + 10 \, S_n + S_{n-1}) + O(h^6)$

5.2 Direct Integration of boundary value problem:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\Phi}{dr}\right) = -4\pi\rho$$

$$\Phi(r) = r^{-1}\phi(r)$$

$$\frac{d^2\phi}{dr^2} = -4\pi r\rho$$

- $K^2=0$, $S=4\pi\rho r$, if $\rho(r) = 1/8\pi\ e^{-r}$
- Exact solution for the problem:
- $\Phi(r) = 1 - ½\,(r + 2)\,e^{-r}$, from which
- $\Phi = \varphi\, r^{-1}$, $S = 4\pi\rho r = -1/2\, r\, e^{-r}$, so
- $\varphi_{n+1} = 2\varphi_n - \varphi_{n-1} + h^2/12(S_{n+1}+10S_n+ S_{n-1})$

EXAMPLE 5.1

- Write a FORTRAN program to solve for $\Phi(r)$ numerically and compare with the analytical solution?

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\Phi}{dr}\right) = -4\pi\rho$$

$$\Phi(r) = r^{-1}\phi(r)$$

$$\frac{d^2\phi}{dr^2} = -4\pi r\rho$$

PROGRAM 5.1

```
•        DIMENSION PHI(0:200)
•        EXACT(R)=1.-(R+2)*EXP(-R)/2
•        SOURCE(R)=-R*EXP(-R)/2
•         H=.1
•         NSTEP=20./H
•         CONST=H**2/12
•         SM=0.
•        SZ=SOURCE(H)
•        PHI(0)=0
•        PHI(1)=EXACT(H)
•        DO 10 IR=1,NSTEP-1
•        R=(IR+1)*H
•        SP=SOURCE(R)
•         PHI(IR+1)=2*PHI(IR)-PHI(IR-1)+CONST*(SP+10.*SZ+SM)
•            SM=SZ
•            SZ=SP
•            DIFF = EXACT (R ) – PHI (IR)
•           PRINT *, R,EXACT(R),PHI(IR),DIFF
  10        CONTINUE
•           STOP
•            END
```

•5.3 Green`s Function solution of boundary value problem:

- The potential from charge distribution of multiple order $l > 0$,

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right) \phi = -4\pi\rho$$

- Which has two solution (homogeneous)
- $\Phi = r^{l+1}$, $\Phi = r^{-l}$,
- these two solutions have two different behaviors so it is to find r_m that permits satisfactory integration of inner and outer potential B.C. $\Phi(x=0) = \Phi(x=\text{infinity}) = 0$

•Introducing the Green function to the solution,

$$\phi(x) = \int_0^\infty G(x, x`)\, S(x`)\, dx$$

- Where G green function satisfying,

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

$$\frac{dG}{dx} /_{x = x' + \varepsilon} - \frac{dG}{dx} /_{x = x' - \varepsilon} = 1$$

- For x not equal x `, to find G, consider two solution $\Phi_<$ and $\Phi_>$, satisfying the boundary conditions x=0 and x= infinity respectively and normalized so that their Wroniskian W is Unity

- $$W = \frac{d\phi_{\succ}}{dx}\phi_{\prec} - \frac{d\phi_{\prec}}{dx}\phi_{\succ}$$

then the Green function is,

- $G(x,x`)= \Phi_{<}(x_{<})\ \ \Phi_{>}(x_{>})$, $x_{<}$ and $x_{>}$ are the smallest and largest of x and x` respectively. Then,

$$\phi_{<}(x)=\phi_{>}(x)\int_{0}^{x}\phi_{<}(x')S(x')dx'+\phi_{<}(x)\int_{0}^{\infty}\phi_{>}(x')s(x)'dx'$$

- Analytical solution: $\Phi_{<} = r^{l+1}$ and
- $\Phi_{>}{}^{= 1/2l+1}\ r^{-l}$,

•5.4 Eigen values of the wave equation:

- $0<x<1$, φ transverse displacement of string
- K constant wave number,

$$\frac{d^2\phi}{dx^2} = -k^2\phi, (\phi(x=0) = \phi(x=1) = 0)$$

- The eigen function and eigen values of the problem, $\varphi_n = \sin K_n x$, $K_n = n\pi$,
- SHOOTING METHOD: integrate for each k, from x=0 with initial condition $\varphi(x=0)=0$, $\varphi`(x=0)=\delta$, the number δ can be chose arbitrary

Upon integrating to x=1, we will find non vanishing value φ, so k will be real just untill

we find φ(x=1)=0 within an error, the problem of finding values of k for which φ vanishes is root finding problem of chapter 3.

- Example 5.2: Write program to find the lowest eigen values of stretched string by the shooting method described above?

$$\frac{d^2\phi}{dx^2} = -k^2\phi, (\phi(x=0) = \phi(x=1) = 0)$$

```
•       REAL K
•        K=1.
•        DK=1.
•         TOLK=1.E-05
•         CALL INTGRT(K,PHIP)       PHIOLD=PHIP
  10      CONTINUE
•         K=K+DK
•         CALL INTGRT(K,PHIP)
•          IF (PHIP*PHIOLD .LT. 0) THEN
•            K=K-DK
•            DK=DK/2
•           END IF
•          IF (ABS(DK) .GT. TOLK) GOTO 10
         EXACT=4.*ATAN(1.)
•        PRINT *, ' eigenvalue, error =',K,EXACT-K
         STOP
•       END
```

```
SUBROUTINE INTGRT(K,PHIP)
      REAL K
    DATA NSTEP/100/
          H=1./NSTEP
      PHIM=0.
     PHIZ=.01
      CONST=(K*H)**2/12.
      DO 10 IX=1,NSTEP-1
      PHIP=2*(1.-5.*CONST)*PHIZ -(1.+CONST)*PHIM
PHIP=PHIP/(1+CONST)
       PHIM=PHIZ
       PHIZ=PHIP
10     CONTINUE
     PRINT *, K,PHIP
     RETURN
    END
```

•5.5 Stationery solution of one dimensional Schrodinger equation:

- The time dependent Schrodinger equation for a particle of mass m in a potential V(x),

$$\frac{d^2\psi}{dr^2} + K^2(x)\psi(x) = 0$$

$$\psi(x_{\min}) = \psi(x_{\max}) = 0$$

$$K^2(x) = \frac{2m}{\hbar^2}(E - V(x)) = 0$$

- This equation can be solve using the shooting method x_m turning point.

$$\psi_< = \psi_>$$

$$\frac{d\psi_<}{dx} - \frac{d\psi_>}{dx}\Big|_{x=x_m} = o$$

- Which can be approximated,

$$f = \frac{1}{\psi}\left(\psi_<(x_m - h) - \psi_>(x_m - h)\right) = 0$$