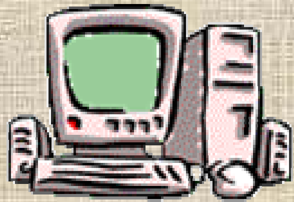

COMPUTATION PHYSICS

PHYS 6312

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CHAPTER 6

Special Function and Gaussian Quadrature

- 6.1 Special Function:
- (a) Lavenders Polynomial, P_L (x)
- For |x|< or equal 1, L =0,1,2
- Solution of Schrodinger equation, angular part leads to recursion relation,
- $(L+1)P_{L+1}(x) + L\, P_{L-1}(x)\ (2L+1)xP_L(x)=0$, $P_0(x)= 1$, $P_1(x)=x$ using above equation we can calculate any higher order of L
- example 6.1 for x calculate P_L (x) ?

Program 6.1

```
•   20   PRINT *, ' Enter x, l (l .lt. 0 to stop)'
•        READ *, X,L
•        IF (L .LT. 0) THEN        STOP
•        ELSE
•        IF (L .EQ. 0) THEN
•        PL=0.
•        ELSE IF (L .EQ. 1) THEN
•        PL=X
•        ELSE
•          PM=1.
•          PZ=X
•        DO 10 IL=1,L-1
•           PP=((2*IL+1)*X*PZ-IL*PM)/(IL+1)
•           PM=PZ
•             PZ=PP
•   10       CONTINUE
•             PL=PZ
•           END IF
•           PRINT *,X,L,PL
•           GOTO 20
•             END
```

•(b) Cylinderical Bessel Function $J_n(x)$ and $Y_n(x)$:

- Which arise from regular and irregular solution of the wave equation, these function satisfy recursion relation :
- $C_{n-1}(x) - C_{n+1} = (2n/x)\, C_n(x)$
- Where $C_n(x)$ either $J_n(x)$ or $Y_n(x)$ to get higher order we need C_0 and C_1.
- Which can be obtained from polynomial approximation $J_0(x)=x^{-1/2} f_0 \cos\theta$

$$Y_0(x) = x^{-1/2} f_0 \sin\theta$$

•(f_0 and θ are constant), previous equation can be written if we subtract 2 C_n, then

- $C_{n+1} - 2\,C_n + C_{n-1} = 2\,(\,n/2 - 1\,)\,C_n$
- Also from normalization,

- $J_0(x) + 2\,J_2(x) + 2\,J_4(x) + \ldots = 1$

- Example 6.2:Write FORTRAN program to evaluate the regular cylindrical Bessel Function backward recursion?

Program 6.2

```
REAL J(0:50)100   PRINT *, ' Enter maximum value of n (.le. 50; .lt. 0 to stop)'
READ *, NMAX
 IF (NMAX .LT. 0) STOP
 IF (NMAX .GT. 50) NMAX=50
 PRINT *,' Enter value of x'
 READ *,X
J(NMAX)=0.
  J(NMAX-1)=1.E-20
  DO 10 N=NMAX-1,1,-1
  J(N-1)=(2*N/X)*J(N)-J(N+1)
10   CONTINUE
 SUM=J(O)
  DO 20 N=2,NMAX,2
   SUM=SUM+2*J(N)
20      CONTINUE
  DO 30 N=0,NMAX
J(N)=J(N)/SUM
   PRINT *,N,J(N)
30   CONTINUE
 GOTO 100
 END
```

•The regular and irregular spherical Bessel function, j_l and n_l satisfy the recursion relation

$$S_l + S_{l-1} = (2l+1)/x \quad S_l$$

- Where S_l is either j_l and n_l , $J_0(x) = \sin x / x$
- $j_1(x) = \sin x/x^2 - \cos x / x$
- $j_2(x) = (3/x^3 - 1/x) \sin x - 3/x^2 \cos x$
- $n_0(x) = - \cos x/x$, $n_1 = -\cos x/x^2 - \sin x / x$
- $n_2(x) = (-3/x^3 + 1/x) \cos x - 3/x^2 \sin x$

•6.2 Gaussian quadrature :

- Consider the problem of evaluation of ,

$$I = \int_{-1}^{1} f(x)\,dx$$

let

$$I \approx \sum_{n=1}^{N} W_n f(x_n)$$

$$x_n = -1 + 2\frac{n-1}{N-1}$$

- Equally spaced lattice points for TR, S, quadrature

- For Simpson`s rule: $\int_{-h}^{h} f(x)dx = \frac{h}{3}(f_1 + 4f_0 + f_{-1})$

- N=3, x_1 = -1, x_2 =0 , x_3 = 1, w_1 =w_3 =1/3,
- W_2 =4/3, this formula is exact for polynomial degree 3 or less. For a polynomial of N-1 degree,

$$\int_{-1}^{1} x^p dx = \sum_{n-1}^{N} w_n x_n{}^p ; p = 0,1,..., N-1$$

- Consider Lagendere polynomial,

$$\int_{-1}^{1} p_i(x) P_j(x) dx = \frac{2}{2i+1} \partial_{ij}$$

•A Polynomial of degree 2N-1 or less can be written as, $f(x) = Q(x)\, P_N(x) + R(x)$

- Then, $\int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} (QP_n + R)\,dx$

$$= \int_{-1}^{1} R\,dx$$

$$I = \sum_{n=1}^{N} w_n \left(Q(x_n)\, P_N(x_n) + R(x_n)\right)$$

$$= \sum_{n=1}^{N} w_n$$

$$w_n = \frac{2}{(1 - x_n^2)(P_N^l(x_n))^2}$$

This is known Gauss lagendere quadrature formula if x in (a,b) change variable to t

$$t = -1 + 2\frac{x - Q}{b - a}$$

$$\int_0^{\infty} e^{-x} f(x)\,dx \approx \sum_{n=1}^{N} w_n f(x_n)$$

$$\int_{-\infty}^{\infty} e^{-x^2} f(x)\,dx$$

•Example:Evaluate the integral using 3-point Gauss Legendere quadrature Change variable from t to x,

$$I = \int_0^3 (1+t)^{1/2}\,dt = 4.6667$$

$$x = -1 + \frac{2}{3}t$$

$$I = \frac{3}{2}\int_{-1}^{1}\left(\frac{3}{2}x + \frac{5}{2}\right)^{1/2} dx$$

- For N=3, the weights, x_1 =- x_3 =0.774597
- x_2=0, w_1=w_3=0.555556,w_2=.88889

$$\int_{-1}^{1}(1-x^2)^{1/2}\,dx = \frac{\pi}{2}$$

$$\int_{-1}^{1}(1-x^2)^{1/2} f(x)\,dx = \sum_{n=1}^{N} w_n f(x_n)$$

$$x_n = \cos\frac{n}{N+1}\pi \qquad w_n = \frac{\pi}{N+1}\sin^2\frac{n}{N+1}\pi$$

Chapter 7
Matrix Operation

- Matrix addition, subtraction, multiplication
- And Eigen values problems
- $A_{i,j}$ and $B_{i,j}$
- $a_{1,1}, a_{1,2}, a_{1,3}, \ldots..$
- $b_{1,1}, b_{1,2}, b_{1,3}, \ldots.$
- $A+B = \sum_{i=1}^{n} \sum_{j=1}^{m} (a_{i,j} + b_{i,j})$

$$AxB = \sum (a_{ik} b_{k,j})$$

Example 7.1

- Write Program to calculate the sum, subtraction, and multiplication of two matrices A and B of different rows and coulomns?

Chapter 8
Monte Carlo Methods

- System with large number of degrees of freedom are very important in physics.
- The number of atoms, electrons, molecules. System containing this large numbers would involve the evaluation integrals of very high dimension. The name of Monte Carlo comes from random or chance.
- Random Number Generators in Computer

•The basic Monte Carlo Strategy:

- The Power of M. C. M. is in evaluation multidimensional situation, simply we explain the one-dimensional method, the integral I can be evaluated as:

$$I = \int_0^1 f(x)\,dx$$

- The average of f over the region 0 to 1 is:

$$I \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

•The average of f evaluated over N values of x_i

- The error associated with this quadrature, variance is :

$$\sigma_I^{\,2} \approx \frac{1}{N}\sigma^2{}_f = \frac{1}{N}\left[\frac{1}{N}\sum_{i=1}^{N} f_i^{\,2} - \left(\frac{1}{N}\sum_{i=1}^{N} f_i^{\,2}\right)^2\right]$$

- Measures the extend to which f deviates from its average values over the region of integration. Example : Use Monte Carlo to evaluate the integral,

$$\int_0^1 \frac{dx}{1+x^2} = \frac{\pi}{4} = 0.78540$$

- INTEGER SEED
- DATA SEED/987654321/
- DATA EXACT/.78540/
- FUNC(X)=1./(1.+X**2)10
- PRINT *, ' Enter number of points (0 to stop)' READ *, N
- IF (N .EQ. 0) STOP
- SUMF=0.
- SUMF2=0.
- DO 20 IX=1,N
- FX=FUNC(RAN(SEED))
- SUMF=SUMF+FX
- SUMF2=SUMF2+FX**2
- 20 CONTINUE
- FAVE=SUMF/N
- F2AVE=SUMF2/N
- SIGMA=SQRT((F2AVE-FAVE**2)/N)
- PRINT *,' integral =',FAVE,' +- ',SIGMA,' error = ',EXACT-FAVE
- GOTO 10
- END