APPENDIX A

MATHEMATICAL RELATIONS

A.1 Stirling Numbers of the First Kind[28]

The operations for reducing factorial to polynomials and vice versa are facilitated by use of Stirling numbers which we now discuss.

The factorial polynomial of degree n

$$x^{(n)} = x(x-1)(x-2)\ldots(x-n+1) \qquad \text{(A.1.1)}$$

plays a role in the finite calculus similar to that played by x^n in the infinitesimal calculus. Since

$$x^{(n)} = x^{(m)} (x-m)^{(n-m)} \quad , m < n$$

it is convenient, in order that this equation hold for $m = 0$, to define $x^{(0)}$ to be 1. Evidently $x^{(m)}$ equal zero for $x = 0,1,2,\ldots,(n-1)$, whereas if x is an integer greater than $(n-1)$, we may write

$$x^{(n)} = \frac{x!}{(x-n)!}$$

If the multiplication on the right in (A.1.1) is performed, a polynomial of degree n in x will result. Thus, $x^{(n)}$ may be written

$$x^{(n)} = S_1^n x + S_2^n x^2 + S_3^n x^3 + \ldots + S_n^n x^n$$

$$= \sum_{i=1}^{n} S_i^n x^i \qquad \text{(A.1.2)}$$

The upper index of S_i^n is the degree of the polynomial under consideration and the lower index is that of the power of x with which it is associated.

The number S_i^n are called Stirling numbers of the first kind.

Thus

$$x^{(n)} = \sum_{i=1}^{n} S_i^n x^i$$

and

$$x^{(n+1)} = \sum_{i=1}^{n+1} S_i^{n+1} x^i$$

But $$x^{(n+1)} = x^{(n)} (x-n)$$

and from (A.1.2)

$$x^{(n+1)} = x^{(n)} (x-n) = \sum_{i=1}^{n} S_i^n x^i (x-n)$$

Therefore

$$\sum_{i=1}^{n+1} S_i^{n+1} x^i = \sum_{i=1}^{n} S_i^n x^i (x-n)$$

By equating coefficients of x^i in the above equation, noting that

$$(S_{i-1}^n x^{i-1} + S_i^n x^i)(x-n)$$

contains two terms in x^i, we have the recurrence relation

$$S_i^{n+1} = S_{i-1}^n - nS_i^n \qquad \text{(A.1.3)}$$

Also, by equating coefficient, we get $S_o^n = o$ and $S_n^n = 1$. Further, $S_i^n = 0$ if $i > n$. Applying (A.1.3) we have, for examples,

$$S_1^2 = S_0^1 - S_1^1 = 0 - 1 = -1,$$

$$S_2^2 = S_1^1 - S_2^1 = 1 - 0 = 1,$$

$$S_1^3 = S_0^2 - 2S_1^2 = 0 - 2(-1) = 2,$$

$$S_2^3 = S_1^2 - 2S_2^2 = -1-2(1) = -3$$

A table of these numbers is easily constructed.

Table A.1.1 Stirling numbers of the first kind

n \ S_i^n	S_1^n	S_2^n	S_3^n	S_4^n	S_5^n	S_6^n	S_7^n
1	1						
2	-1	1					
3	2	-3	1				
4	-6	11	-6	1			
5	24	-50	35	-10	1		
6	-120	274	-225	85	-15	1	
7	720	-1764	1624	-735	175	-21	1

Using formula (A.1.3) any entry in the table is the number above and to left minus the product of the number immediately above and the number n in that row. Thus

$$-225 = -50 - 5(35)$$

$$274 = 24 - 5(-50)$$

If we put x = 1 in (A.1.2) we obtain, $(n > 1)$,

$$S_1^n + S_2^n + S_3^n + \ldots + S_n^n = \sum_{i=1}^{n} S_i^n = 0 \qquad (A.1.4)$$

That is, the sum of the number in each row of the table is equal to zero. This fact can serve as a check in constructing the table.

With the table at hand we can immediately write down the polynomial that is equal to any factorial whose form is $x^{(n)}$. Thus

$$x^{(6)} = x^6 - 15x^5 + 85x^4 - 225x^3 + 274x^2 - 120x$$

A.2 Stirling Numbers of the Second Kind[20]

The Stirling numbers of the second kind connects the power to the factorial, i.e.

$$x^n = \sum_{k=0}^{n} S(n,k)\, x^{(k)} \qquad (A.2.1)$$

where

$$x^{(k)} = x(x-1)(x-2)\ldots(x-k+1)$$

$$x^n = S(n,0)x^{(0)} + S(n,1)x^{(1)} + \ldots + S(n,n)x^{(n)}$$

The recursion relation between the Stirling numbers of the second kind can be established as follows

$$x^{n+1} = \sum_{k=0}^{n+1} S(n+1,k)\, x^{(k)} \qquad (A.2.2)$$

But $x^{n+1} = x^n \cdot x$,

and from (A.2.1)

$$x^{n+1} = x^n . x = \sum_{k=0}^{n} S(n,k)\, x^{(k)} . x \qquad (A.2.3)$$

Since

$$\sum_{k=0}^{n} S(n,k)\, x^{(k)} . x = \sum_{k=0}^{n} S(n,k) x^{(k)} . x - \sum_{k=0}^{n} kS(n,k) x^{(k)} + \sum_{k=0}^{n} k\, S(n,k) x^{(k)}$$

$$= \sum_{k=0}^{n} S(n,k) x^{(k)} (x-k) + \sum_{k=0}^{n} kS(n,k) x^{(k)}$$

Then (A.2.3) becomes

$$x^{n+1} = \sum_{k=0}^{n} S(n,k) x^{(k)} (x-k) + \sum_{k=0}^{n} k\, S(n,k) x^{(k)}$$

$$= \sum_{k=0}^{n} S(n,k) x^{(k+1)} + \sum_{k=0}^{n} k\, S(n,k) x^{(k)} \qquad (A.2.4)$$

From (A.2.2) and (A.2.4), we get

$$\sum_{k=0}^{n+1} S(n+1,k)\, x^{(k)} = \sum_{k=0}^{n} S(n,k) x^{(k+1)} + \sum_{k=0}^{n} kS(n,k) x^{(k)}$$

$$= \sum_{k'=1}^{n} S(n,k'-1)\, x^{(k')} + \sum_{k=0}^{n} k\, S(n,k) x^{(k)}$$

By equating coefficients of $x^{(k)}$ in the above equation, we get

$$S(n+1, k) = S(n,k-1) + k\,S(n,k), \quad k \neq 0,\ k \neq n+1$$

$$S(n,-1) = 0, \quad S(n, n+1) = 0$$

A.3 Generating Function of Stirling Numbers of the Second Kind[29]

The number of ways of putting r different balls in n different cells such that m cells are not empty while the remaining are empty is

$$\binom{n}{m} \sum_{j=0}^{m} \binom{m}{j} (-1)^j (m-j)^r \qquad (A.3.1)$$

Proof : Suppose that the first m cells are not empty. Then the symbolic generating function is

$$(x_1 t + x_1^2 \frac{t^2}{2!} + \ldots)(x_2 t + x_2^2 \frac{t^2}{2!} + \ldots) \ldots (x_m t + x_m^2 \frac{t^2}{2!} + \ldots)$$

(A.3.2)

The number of ways that this can be done is the coefficient of $t^r/r!$ in the above expansion when we set $x_1 = x_2 = \ldots = x_m = 1$. For $x_i = 1$, (A.3.2) reduces to $(e^t - 1)^m$. The same generating function is obtained no matter which m cells are chosen. Since m cells can be chosen from n cells in $\binom{n}{m}$ ways, the required generating function is $\binom{n}{m} (e^t - 1)^m$.

Expanding in powers of t^r yields

$$\binom{n}{m}(e^{t}-1)^{m} = \binom{n}{m}\sum_{j=0}^{m}\binom{m}{j}(-1)^{j}\ e^{(m-j)t}$$

$$= \binom{n}{m}\sum_{r=0}^{\infty}\sum_{j=0}^{m}(-1)^{j}\binom{m}{j}(m-j)^{r}\frac{t^{r}}{r!}$$

Hence we sec that the coefficient of $\frac{t^r}{r!}$ is just (A.3.1).

Equation (A.3.1) is frequently written in terms of Stirling numbers of the second kind, $S(r,m)$ defined by

$$S(r,m) = \frac{1}{m!}\sum_{j=0}^{m}(-1)^{j}\binom{m}{j}(m-j)^{r}\ ,\ r \geq m \qquad (A.3.3)$$

Using (A.3.3), (A.3.1) becomes

$$n(n-1)\ldots(n-m+1)\ S(r,m)$$

A.4 Connection Between $P_n(c)$ Function and Stirling Numbers

If we define a generating function of $P_n(c)$ by

$$g(x;\ c) = \sum_{n=1}^{\infty} P_n(c)\frac{x^n}{n!} \qquad (A.4.1)$$

Then the analysis is considerably simplified, because it can be shown that $g(x;c)$ becomes

$$g(x\ ;c) = \ln(1-c+ce^{x}) \qquad (A.4.2)$$

The above relation (A.4.2) can be considered as the generating function of a distribution in which the probability a number being 1 is c and the probability of being 0 is (1-c).

Thus $$\ln(1-c+ce^{x}) = \sum_{n=1}^{\infty} P_n(c)\frac{x^n}{n!} \qquad (A.4.3)$$

Let $$P_n(c) = \sum_{\ell=1}^{n} A_\ell^n \cdot c^\ell$$

$$= \sum_{\ell=1}^{\infty} A_\ell^n \; c^\ell \quad ; \qquad (A.4.4)$$

$$A_\ell^n = 0, \quad \ell > n$$

Substitute (A.4.4) into (A.4.3), we get

$$\ell n(1-c+ce^x) = \sum_{n=1}^{\infty} \sum_{\ell=1}^{\infty} A_\ell^n \; c^\ell \; \frac{x^n}{n!}$$

$$= \sum_{\ell=1}^{\infty} \left(\sum_{n=1}^{\infty} A_\ell^n \; \frac{x^n}{n!} \right) c^\ell$$

$$\frac{\partial^m}{\partial c^m} \ell n(1-c+ce^x) \Big|_{c=0} = \frac{\partial^m}{\partial c^m} \sum_{\ell=1}^{\infty} \left(\sum_{n=1}^{\infty} A_\ell^n \frac{x^n}{n!} \right) c^\ell \Big|_{c=0} \qquad (A.4.5)$$

$$\frac{\partial^m}{\partial c^m} \ell n(1-c+ce^x) \Big|_{c=0} = \frac{\partial^m}{\partial c^m} \ell n \{1+c(e^x-1)\} \Big|_{c=0}$$

$$= \frac{(-1)^{m-1}(m-1)!}{\{1+c(e^x-1)\}^m} (e^x-1)^m \Big|_{c=0}$$

$$= (-1)^{m-1} (m-1)!(e^x-1)^m \qquad (A.4.6)$$

since $(e^x-1)^m$ is the generating function of Stirling numbers,

$$(e^x-1)^m = m! \sum_{\ell=1}^{m} S(\ell,m) \frac{x^\ell}{\ell!} \qquad (A.4.7)$$

Substitute (A.4.7) into (A.4.6), (A.4.6) becomes

$$\frac{\partial^m}{\partial c^m} \ln(1-c+ce^x) \Big|_{c=0} = (-1)^{m-1} (m-1)!\, m! \sum_{\ell=1}^{m} S(\ell,m) \frac{x^\ell}{\ell!} \; ; \qquad (A.4.8)$$

$$S(\ell,m) = 0, \quad m > \ell$$

$$\frac{\partial^m}{\partial c^m} \sum_{\ell=1}^{\infty} \Big(\sum_{n=1}^{\infty} A_\ell^n \frac{x^n}{n!} \Big) c^\ell \Big|_{c=0}$$

$$= \sum_{\ell=m}^{\infty} \Big(\sum_{n=1}^{\infty} A_\ell^n \frac{x^n}{n!} \Big) c^{\ell-m} \, \ell(\ell-1)(\ell-2)\ldots(\ell-m+1) \Big|_{c=0}$$

$$= \sum_{n=1}^{\infty} A_m^n \frac{x^n}{n!} m! \qquad (A.4.9)$$

Substitute (A.4.8) and (A.4.9) into (A.4.5), we get

$$(-1)^{m-1} (m-1)!\, m! \sum_{\ell=1}^{\infty} S(\ell,m) \frac{x^\ell}{\ell!} = \sum_{n=1}^{\infty} A_m^n \frac{x^n}{n!} m!$$

By equating coefficients of x^n in the above equation, we get

$$A_m^n = (-1)^{m-1} (m-1)! \; S(n,m)$$

and from (A.4.4)

$$P_n(c) = \sum_{m+1}^{\infty} (-1)^{m-1} (m-1)! \; S(n,m) \, c^m$$

APPENDIX B

COMPUTER PROGRAMS

B.1 Density of States

To calculate the density of states, we must know the minimum energy. The following statements in the program for calculating the density of states accomplish after the task of finding the minimum energy

```
      DO  5I = 1, 165
    5 NCOUNT(I) = 0
      II = EK(I,J)
      K = IABS(-84-II) + 1
      IF(EK(I,J).GT.0.0)K = 85+II+1
      NCOUNT(K) = NCOUNT(K) + 1
      WRITE(3,45)
      WRITE(3,35) NCOUNT
```

The important notations in the program are

EK(I,J) $\longrightarrow$ $E(\vec{k})$

NCOUNT $\longrightarrow$ $\rho_o(E')$

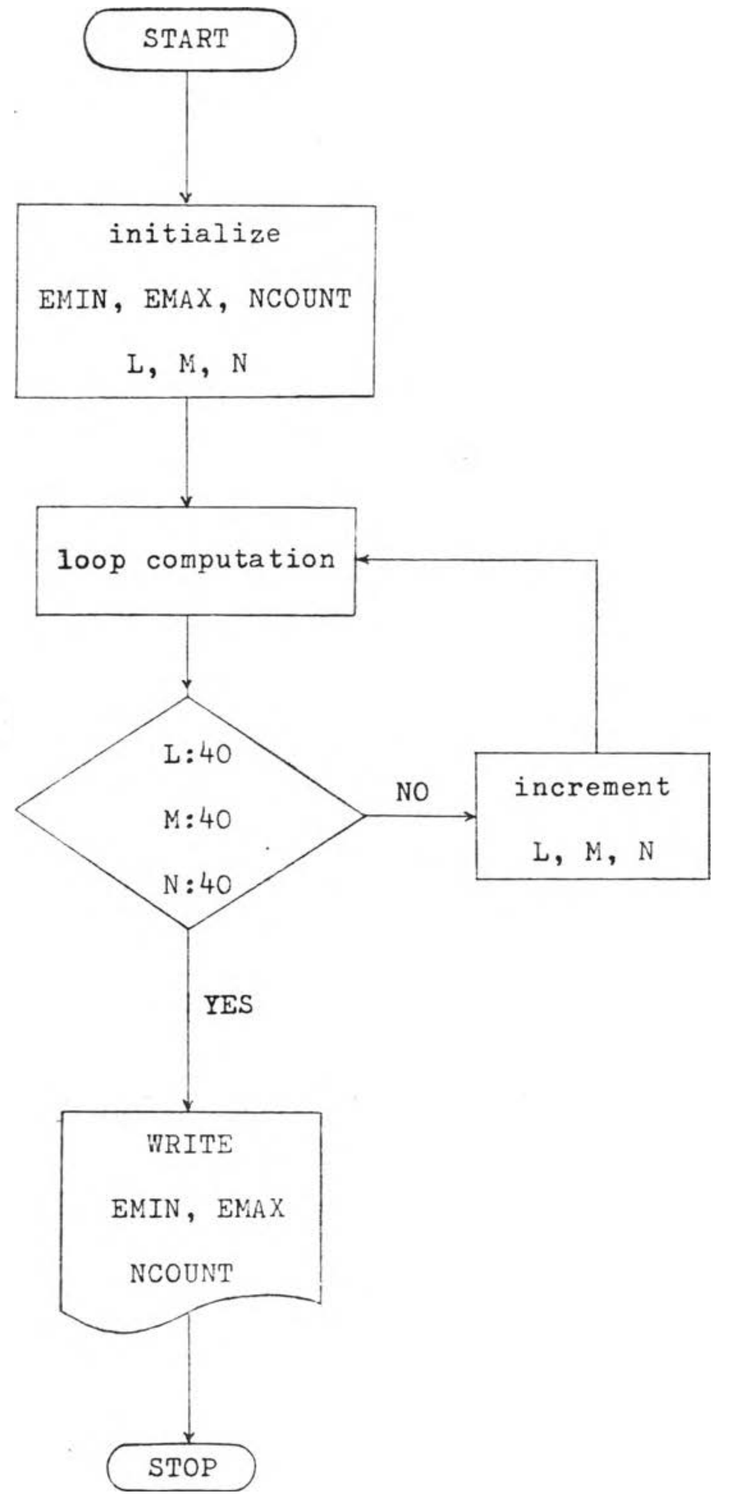
EMIN $\longrightarrow$ E_{min}

EMAX $\longrightarrow$ E_{max}

The complete program is

```
C     EXCITON BAND STRUCTURE
      DIMENSION EK(80,80),NCOUNT(165)
      DATA AM,BM,CM,ACM,ABM,ABCM/-0.6,-3.9,6.1,-3.7,18.0,2.0/
      PI=3.1415926536
      EMIN=1000
      EMAX=-1000
      DO5I=1,165
    5 NCOUNT(I)=0
    1 READ(1,10)MM,NN
      IF(MM.EQ.0) GO TO 20
      DO300KK=MM,NN
      N=-41+KK
      IF(KK.GE.41)N=N+1
   70 DO200J=1,80
      M=-41+J
      IF(J.GE.41)M=M+1
   60 DO100I=1,80
      L=-41+I
      IF(I.GE.41)L=L+1
      A=2.0*PI*FLOAT(L)/40.0
      B=2.0*PI*FLOAT(M)/40.0
      C=2.0*PI*FLOAT(N)/40.0
      D=A/2.0
      E=B/2.0
      EK(I,J)=2.0*(AM*COS(A)+BM*COS(B)+CM*COS(C))+2.0*ACM*
     *(COS(A)*COS(C)-SIN(A)*SIN(C))+4.0*(ABM*COS(D)*COS(E)
     *+ABCM*(COS(C)*COS(D)*COS(E)-SIN(C)*SIN(D)*COS(E)))
      IF(EMIN.GT.EK(I,J))EMIN=EK(I,J)
      IF(EMAX.LT.EK(I,J))EMAX=EK(I,J)
      II=EK(I,J)
      K=IABS(-84-II)+1
      IF(EK(I,J).GT.0.0)K=85+II+1
      NCOUNT(K)=NCOUNT(K)+1
  100 CONTINUE
  200 CONTINUE
  300 CONTINUE
      GO TO 1
   20 WRITE(3,15)EMIN
      WRITE(3,25)EMAX
      WRITE(3,45)
      WRITE(3,35)NCOUNT
   10 FORMAT(2I5)
   15 FORMAT(1H1,10X,'THE MINIMUM ENERGY IS',F10.1/)
   25 FORMAT(11X,'THE MAXIMUM ENERGY IS',F10.1//)
   35 FORMAT(3X,16I8)
   45 FORMAT(11X,'THE DENSITY OF STATE ARE'//)
      STOP
      END
```

Flow chart B.1



B.2 Curve Fitting

We use the HP-97 Programmable Printing Calculator for curve fitting. In least squares method for curve fitting, we have 4 x 4 matrix (sec section 4.3). We found that we must calculate the summations of x_i^o , x_i^1 , x_i^2 , ..., x_i^6 and y_i, $x_i y_i$, $x_i^2 y_i$, $x_i^3 y_i$. The program is shown in B.2.1. Later we use Math Pac I of HP-97 for matrix solution. After we solved for a, b, c and d, we can calculate $\rho_o(E')$ by the program as shown in B.2.2. We use Math Pac I of HP-97 for calculating the intesection points of curve.

B.2.1

```
001  *LBLa   21 16 11
002  CLRG       16-53
003     0          00
004  STOA       35 11
005   R/S          51
006  *LBLB      21 12
007  STOC       35 13
008     ÷         -24
009  STOB       35 12
010  RCLC       36 13
011   1/X          52
012  STOD       35 14
013   R/S          51
014  *LBLA      21 11
015  ST+0    35-55 00
016  RCLB       36 12
017     ×         -35
018  ST+1    35-55 01
019  RCLB       36 12
020     ×         -35
021  ST+2    35-55 02
022  RCLB       36 12
023     ×         -35
024  ST+3    35-55 03
025  RCLB       36 12
026  ST+4    35-55 04
027    X²          53
028  ST+5    35-55 05
029  RCLB       36 12
030     ×         -35
031  ST+6    35-55 06
032  RCLB       36 12
033     ×         -35
034  ST+7    35-55 07
035  RCLB       36 12
036     ×         -35
037  ST+8    35-55 08
038  RCLB       36 12
039     ×         -35
040  ST+9    35-55 09
041  RCLA       36 11
042     1          01
043     +         -55
044  STOA       35 11
045  RCLB       36 12
046  RCLD       36 14
047     +         -55
048  STOB       35 12
049   R/S          51
050  *LBLC      21 13
051  RCLA       36 11
052  PRTX         -14
053  RCL4       36 04
054  PRTX         -14
055  RCL5       36 05
056  PRTX         -14
057  RCL6       36 06
058  PRTX         -14
059  RCL7       36 07
060  PRTX         -14
061  RCL8       36 08
062  PRTX         -14
063  RCL9       36 09
064  PRTX         -14
065   SPC       16-11
066  RCL0       36 00
067  PRTX         -14
068  RCL1       36 01
069  PRTX         -14
070  RCL2       36 02
071  PRTX         -14
072  RCL3       36 03
073  PRTX         -14
074   R/S          51
```

B.2.2

```
001  *LBLA      21 11
002  ENT↑         -21
003  ENT↑         -21
004  ENT↑         -21
005  RCLD       36 14
006     ×         -35
007  RCLC       36 13
008     +         -55
009     ×         -35
010  RCLB       36 12
011     +         -55
012     ×         -35
013  RCLA       36 11
014     +         -55
015   RTN          24
016  *LBLB      21 12
017  STO0       35 00
018    R↓         -31
019  STO1       35 01
020  *LBL1      21 01
021  RCL1       36 01
022   SPC       16-11
023  PRTX         -14
024  GSBA       23 11
025  PRTX         -14
026  RCL0       36 00
027  RCL1       36 01
028  X=Y?       16-33
029   R/S          51
030     1          01
031  ST+1    35-55 01
032  GTO1       22 01
033   R/S          51
```

B.3 Integration

In this integration program, we use the Newton-Cctes open type 5 points formula. The expression which we will evaluate is (the left side are the notation in program)

$$SUM = \int \frac{\rho_o(E')}{E - E'} dE'$$

Our relation $\rho_o(E')$ as shown in Fig. B.3.1

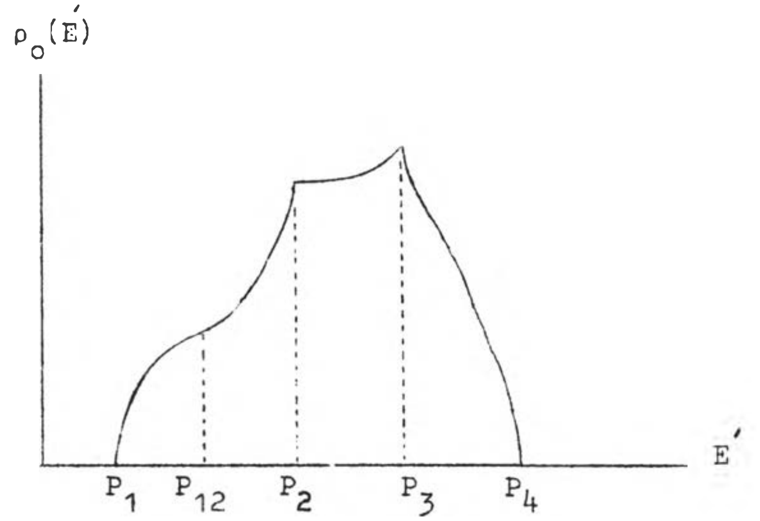


Fig. B.3.1 Show $\rho_o(E')$ and the intervals of integration

When E is out of curve $\rho_o(E')$, we use the interval of integration as shown in Fig. B.3.1

But when E is in curve $\rho_o(E')$, we divide the interval around E have symmetry in two sides of E as shown in Fig. B.3.2. So the total number of intervals is six

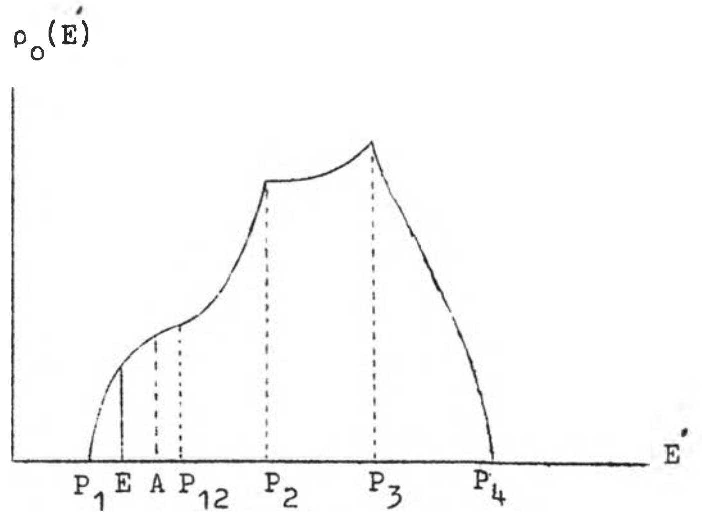


Fig. B.3.2 Show the intervals of integration when E is in curve $\rho_o(E')$

For example, in Fig. B.3.2 we will get

$$A = 2E - P_1$$

For other positions of E, we can evaluate A in the similar way. Some important notations in the program are

$$\text{FINT} \longrightarrow \int_{x_o}^{x_6} f(x)dx = \frac{3h}{10}(11f_1 - 14f_2 + 26f_3 - 14f_4 + 11f_5)$$

$$\text{F} \longrightarrow f(x) = \rho_o(E') / (E - E')$$

The f(x) in our program have three relations which we calculated in section B.2

```
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON  E,A1,B1,C1,D1,A2,B2,C2,D2,A3,B3,C3,D3,P1,P2,P3,P4
      READ (1,20)A1,B1,C1,D1,A2,B2,C2,D2,A3,B3,C3,D3,P1,P2,P3,P4
      READ(1,30) N
      WRITE(3,10)
      WRITE(3,20)A1,B1,C1,D1,A2,B2,C2,D2,A3,B3,C3,D3,P1,P2,P3,P4
      WRITE(3,40)
      P12=P1+(P2-P1)/2.
      I=1
      E=-150.
    5 IF(E.GT.P1.AND.E.LT.P12) GO TO 100
      SUM=FINT(P1,P12,N)
      IF(E.GE.P1.AND.E.LE.P4)  GO TO 300
   15 SUM=SUM+FINT(P12,P2,N)
   25 SUM=SUM+FINT(P2,P3,N)
   35 SUM=SUM+FINT(P3,P4,N)
      GO TO 45
  100 IF(E.GT.(P1+P12)/2.)       GO TO 200
      A=2.*E-P1
      SUM=FINT(P1,A,2*N)
      SUM=SUM+FINT(A,P12,N)
      GO TO 15
  200 IF(E.GT.P12)               GO TO 300
      A=2.*E-P12
      SUM=FINT(P1,A,N)
      SUM=SUM+FINT(A,P12,2*N)
      GO TO 15
  300 IF(E.GT.(P12+P2)/2.)       GO TO 400
      A=2.*E-P12
      SUM=SUM+FINT(P12,A,2*N)
      SUM=SUM+FINT(A,P2,N)
      GO TO 25
  400 IF(E.GT.P2)                GO TO 500
      A=2.*E-P2
      SUM=SUM+FINT(P12,A,N)
      SUM=SUM+FINT(A,P2,2*N)
      GO TO 25
  500 SUM=SUM+FINT(P12,P2,N)
      IF(E.GT.(P2+P3)/2.)        GO TO 600
      A=2.*E-P2
      SUM=SUM+FINT(P2,A,2*N)
      SUM=SUM+FINT(A,P3,N)
      GO TO 35
  600 IF(E.GT.P3)                GO TO 700
      A=2.*E-P3
      SUM=SUM+FINT(P2,A,N)
      SUM=SUM+FINT(A,P3,2*N)
      GO TO 35
  700 SUM=SUM+FINT(P2,P3,N)
      IF(E.GT.(P3+P4)/2.)        GO TO 800
      A=2.*E-P3
      SUM=SUM+FINT(P3,A,2*N)
      SUM=SUM+FINT(A,P4,N)
      GO TO 45
```

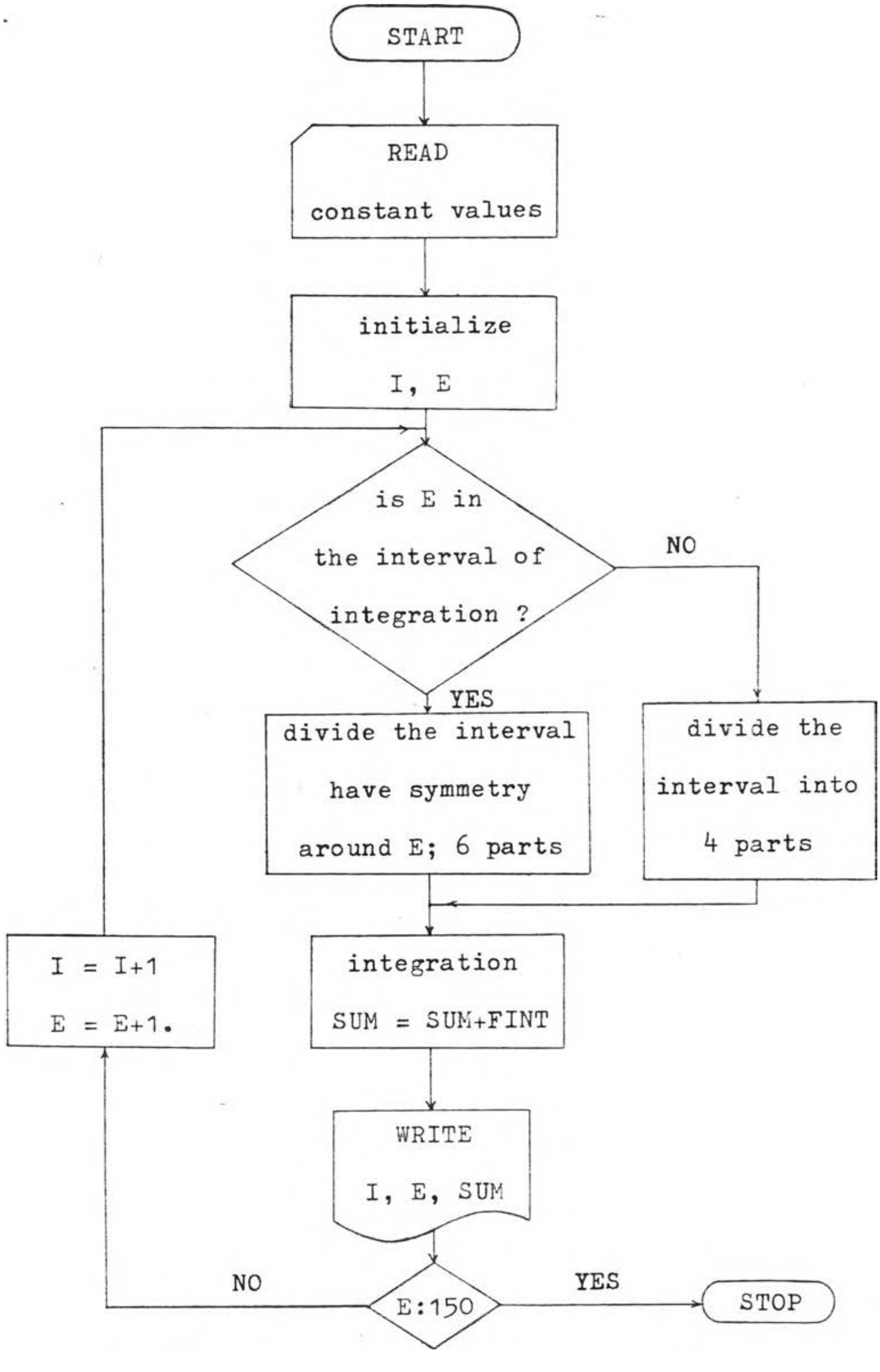
```
  800 A=2.*E-P4
      SUM=SUM+FINT(P3,A,N)
      SUM=SUM+FINT(A,P4,2*N)
   45 R0=SUM
      R2=0.6*SUM
      R4=0.2*SUM
      R6=-0.2*SUM
      R8=-0.6*SUM
      R10=-1.0*SUM
      WRITE(3,50) I,E,R0,R2,R4,R6,R8,R10
      IF(I.EQ.300) GO TO 55
      IF(I/50*50-I.EQ.0) WRITE(3,40)
   55 IF(E.GE.150.) STOP
      I=I+1
      E=E+1.
      GO TO  5
   10 FORMAT(1H1,40X,'DATA')
   20 FORMAT(4E20.9)
   30 FORMAT(I5)
   40 FORMAT(1H1,///65X,'THE RECIPROCAL TRAP DEPTH'
     *,//9X,'I',11X,'E',12X,'C=0.0',12X,'C=0.2',12X
     *,'C=0.4',12X,'C=0.6',12X,'C=0.8',12X,'C=1.0'/)
   50 FORMAT(I10,F15.2,6F17.6)
      END
```

RTRAN IV 360N-FO-479 3-8   FINT   DATE 21/01/81   TIME

```
      REAL FUNCTION FINT*8(A,B,N)
      IMPLICIT REAL*8(A-H,O-Z)
      H=(B-A)/(6*N)
      X=A+H
      FINT=0.
      DO 1 I=1,N
      FINT=FINT+3.*H/10.*(11.*F(X)-14.*F(X+H)+26.*F(X+2.*H)
     *-14.*F(X+3.*H)+11.*F(X+4.*H))
    1 X=X+6.*H
      RETURN
      END
```

```
      REAL FUNCTION F*8(X)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON  E,A1,B1,C1,D1,A2,B2,C2,D2,A3,B3,C3,D3,P1,P2,P3,P4
      IF(X.GE.P1.AND.X.LT.P2) F=(A1+X*(B1+X*(C1+D1*X)))/(E-X)
      IF(X.GE.P2.AND.X.LT.P3) F=(A2+X*(B2+X*(C2+D2*X)))/(E-X)
      IF(X.GE.P3.AND.X.LE.P4) F=(A3+X*(B3+X*(C3+D3*X)))/(E-X)
      RETURN
      END
```

Flow chart B.3



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VITA

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