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N-63-3-1

NOLTR 63-31

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A FORTRAN III (IBM 7090) PROGRAM FOR
THE CALCULATION OF ELECTRON WAVE
FUNCTIONS FOR THE SODIUM ION

NOL

8 FEBRUARY 1963

UNITED STATES NAVAL ORDNANCE LABORATORY, WHITE OAK, MARYLAND

NOLTR 63-31

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NOLTR 63-31
Mathematics Department Report M-34

A FORTRAN III (IBM 7090) PROGRAM FOR
THE CALCULATION OF ELECTRON WAVE FUNCTIONS FOR THE SODIUM ION

Prepared By:
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ABSTRACT: An IBM 7090 program is described. It calculates, using simplified Hartree-Fock equations, the radial parts of the wave functions for the electrons in the sodium ion. Up to 1000 values for each wave function can be calculated. A complete listing of the subroutines and an example is included in this report.

PUBLISHED MARCH 1963

U. S. NAVAL ORDNANCE LABORATORY
WHITE OAK, MARYLAND

NOLTR 63-31

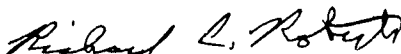
8 February 1963

A FORTRAN III (IBM 7090) PROGRAM FOR THE CALCULATION OF ELECTRON WAVE
FUNCTIONS FOR THE SODIUM ION

This report describes a FORTRAN III (IBM 7090) program for the calculation of sodium-ion wave functions. This has been done in view of future, theoretical evaluations, like transition probabilities and cross sections, which are needed for guidance and interpretation of sodium-arc-tunnel investigations.

This work was performed under NOL Task No. FR-64.

R. E. ODENING
Captain, USN
Commander


RICHARD C. ROBERTS
By direction

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A FORTRAN III (IBM 7090) PROGRAM FOR
THE CALCULATION OF ELECTRON WAVE FUNCTIONS FOR THE SODIUM ION

PURPOSE: Determination of the radial part of the wave functions for the electrons in the 1-s, 2-s and 2-p shells of the sodium ion. The Hartree-Fock equations are used for this in a simplified form, so that one deals with three uncoupled eigenvalue equations. The theory and the application of the results will be discussed in NOLTR 63-32.

METHOD:

A. Mathematical

The following equations are solved for the eigenvalues $\epsilon_1, \epsilon_2, \epsilon_3$ and the eigenfunctions $P(1, r), P(2, r), P(3, r)$:

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r}[y(r) + y_0(1, 1, r)] - \epsilon_1 \right\} P(1, r) = 0$$

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r}[y(r) + y_0(2, 2, r)] - \epsilon_2 \right\} P(2, r) = 0$$

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r}[y(r) + y_0(3, 3, r) + \frac{2}{5} y_2(3, 3, r)] - \epsilon_3 - \frac{2}{r^2} \right\} P(3, r) = 0$$

where $y(r) = 11 - 2y_0(1, 1, r) - 2y_0(2, 2, r) - 6y_0(3, 3, r)$

$$\text{and } y_k(n, m, r) = \int_0^r \left(\frac{\rho}{r}\right)^k P(n, \rho) P(m, \rho) d\rho + \int_r^\infty \left(\frac{r}{\rho}\right)^{k+1} P(n, \rho) P(m, \rho) d\rho$$

with the boundary conditions:

$$r \rightarrow 0 \quad P(1, r) \sim r \quad P(2, r) \sim r \quad P(3, r) \sim r^2$$

$$r \rightarrow \infty \quad P(n, r) \sim e^{-\epsilon_n \cdot r}$$

$$\text{and the normalization condition } \int_0^\infty P^2(n, \rho) d\rho = 1$$

The solutions are obtained by iteration: Starting with a first guess for $\epsilon_1, \epsilon_2, \epsilon_3$ and $P(1, r), P(2, r), P(3, r)$

1) $y(r)$ and $y_k(n, m, r)$ are calculated

- 2) Then new $P(n,r)$ are calculated by integrating the differential equations from $r = 0$ outwards. This is repeated adjusting ϵ_n until the absolute value of $P(n,r)$ is a minimum at an arbitrarily chosen, fixed, large r -value. The changes in ϵ_n are effected as long as they are larger than the required eigenvalue accuracy TE.
- 3) With the new eigenvalues $\epsilon_1, \epsilon_2, \epsilon_3$ and the pertaining new eigenfunctions $P(1,r), P(2,r), P(3,r)$ the calculations are started again in 1).

This is repeated until $\int_0^\infty (P_{old} - P_{new})^2 dr \leq TT$, the prescribed wavefunction accuracy.

Numerical Remarks:

- 1) Since the differential equations do not contain the first derivative, Numerov's integration procedure is used: If the D.E. is $f''(r) = a(r) \cdot f(r) + b(r)$ one can, using $\delta^2 f_j = (\Delta r)^2 [f_j'' + \frac{1}{12} \delta^2 f_j'']$ and $f_{j+1} = 2f_j - f_{j-1} + \delta^2 f_j$, derive

$$f_{j+1} = \frac{f_j [2 + \frac{(\Delta r)^2}{12} \cdot 10 \cdot a_j] + f_{j-1} [-1 + \frac{(\Delta r)^2}{12} a_{j-1}] + \frac{(\Delta r)^2}{12} [10 b_j + b_{j+1} + b_{j-1}]}{1 - \frac{(\Delta r)^2}{12} a_{j+1}}$$

- 2) The preceding formula shows that the numerical procedure is simplified if the values of the independent variable r are equidistant. On the other hand the accuracy is better if $\frac{\Delta r}{r} =$ constant. Therefore as a compromise the r -range is subdivided into several sets and in each of these sets, the r -values are equidistant.

- 3) Since the eigenvalues can be determined numerically only within a certain accuracy, the pertaining wave functions do not decrease exponentially for increasing r , but their absolute values go through a minimum and increase then exponentially. Therefore the final wave functions are obtained by integrating the differential equations, using the final eigenvalues ϵ_n , from $r = 0$ outward and from large r -values inward. The outward and the inward solutions are then matched at some point, which can be prescribed.
- 4) Since $P(3,r)$ enters in $y(r)$ with the coefficient 6, $P(1,r)$ and $P(2,r)$ however only with the coefficient r , the iteration procedure is speeded up by determining first $P(3,r)$.

B. Programming

Input: in the following order

- 1) JF

Format (I3), restriction $JF \leq 20$, 1 card

JF is the number of sets into which the range of the independent variable r is divided. Each of these sets is once more subdivided into equally spaced intervals. The endpoints of these intervals are the values of r used in the program and calculated by the program in the subroutine Radius.

- 2) NF(J) XF(J)

Format (I4, E14.6), restriction: $NF(JS(L)) \geq 6$, $J = 1, \dots, JF$, JF cards

NF(J) is the number of intervals into which the Jth set is subdivided.

XF(J) is the right endpoint of the Jth set

3) JS(L)

Format (3I3), L = 1,...3, 1 card

JS(L) is the number of the r-set in which the backward and the forward integrated solution for the Lth wave function will be matched.

4) TE TT E(1) E(2) E(3)

Format (5E14.6) 1 card

TE is permissible absolute error for eigenvalues.

TT is permissible sum of squared deviations of wave functions.

E(L) is the (guess of the) Lth eigenvalue.

5) P(L,N)

Format (3E14.6), L = 1,...3, N = 1,...NFF

Restriction $NFF \leq 1000$, NFF cards

P(L,N) is the Nth value of the guessed Lth wave function.

NFF is the total number of R-points and will be calculated in Radius.

6) DATE

Format (2A5) 1 card

Output: in the following order

- 1) Each time the calculated eigenvalue E(L) differs from the previous value of E(L) by an amount smaller than TE there will be printed:

a) P(L,N) PB(N)

Format (2E18.9), N = 1,NFF

P(L,N) is the Nth value of the Lth wave function obtained by forward integration.

PB(N) is the Nth value of the Lth wave function obtained by backward integration.

b) E(L)

Format (E18.9)

E(L) the calculated Lth eigenvalue

2) At the end of the complete calculation will be printed:

a) DATE

Format (2A5)

b) E(L)

Format (3E14.9), L = 1,3

E(L) the final values of the eigenvalues

c) TE, TT

Format (2E14.6)

TE is the permissible absolute error for eigenvalues

TT is the permissible sum of squared deviation of wave functions.

d) R(N) P(1,N) P(2,N) P(3,N) Z(N) ZNL(1,N) ZNL(2,N)
ZNL(3,N)

Format (8E14.6), N = 1,NFF

R(N) is the Nth value of the independent variable r

P(L,N) is the Nth value of the final Lth wave function

Z(N) is the Nth value of the sodium ion potential

ZNL(L,N) is the Nth value of the potential for the Lth wave function

PROGRAM FORM:

A. Type of Code FORTRAN 7090

B. Type of Monitor BELL

C. Number of Tape Units required (other than System Tapes): None

CODING INFORMATION:

A. Storage Required

1. Regular: 3894 (Total)

2. Common: 19037 (Total)

B. Accuracy:

TE - The accuracy to which the eigenvalues are to be calculated can be prescribed.

TT - The sum of squared deviations of iterated wave functions can be prescribed.

C. Timing:

It takes about 7 minutes to calculate 70 values for each of the three wave functions, when the prescribed accuracy of the eigenvalues is $TE = 10^{-3}$ and the prescribed sum of squared deviations of iterated wave functions is $TT = 10^{-2}$.

D. Additional Subroutines Required:

This program uses only subroutines on the library tape and subroutines incorporated in this program. In fact this program has been split into the following subroutines:

1) Main Hartree Storage 217 + Common is the Main program.

2) Subroutine BINT(L) Storage 304 + Common. It calculates the Lth wave function by integrating backwards from large r values to small ones.

3) Subroutine EIGEN(L) Storage 283 + Common. It determines the Lth eigenvalue.

4) Subroutine FINT(L) Storage 390 + Common. It calculates the Lth wave function by integrating forward.

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- 5) Subroutine OUTPUT Storage 182 + Common. Prints the final results.
- 6) Subroutine PRINT(L) Storage 41 + Common. Prints for the Lth wave function the values obtained by forward integration as well as the values obtained by backward integration. It also prints the Lth eigenvalue.
- 7) Subroutine RADIUS Storage 59 + Common. Divides the r-range into several sets and covers each of these sets by equidistant points.
- 8) Subroutine RINT(U) Storage 137 + Common. Dimension U(1000) calculates the integral of a function defined on the points calculated in Radius. U are the values of the integral, the function itself is transmitted through Common.
- 9) Subroutine SSRI(L) Storage 244 + Common. Calculates certain integrals of the Lth wave function
- 10) Subroutine TEST Storage 153 + Common. Tests whether the calculated wave functions fulfill the required accuracy.
- 11) Function YB(A,D,L) Storage 128 + Common
Dimension A(10), D(2)
Is a backward interpolation for A, to get from one set of equidistant r-values into the preceding one.
- 12) Function YF(A,D,L) Storage 81 + Common.
Dimension A(7), D(2)
Is a forward interpolation for A, to get from one set of equidistant r-values into the following one.

- 13) Subroutine Y2(P2) Storage 1088 + Common
Dimension P2(1000)
Calculates some integrals of the wave functions.
- 14) Subroutine ZPI Storage 101 + Common. Calculates the
potentials for the wave functions.

USE:

The determination of these wave functions was undertaken in connection with a sodium-arc-tunnel project. With their aid cross-sections, transition-probabilities, line strength and line profiles can be calculated. This in turn can be used for interpretation of experimental data.

SPECIAL FEATURES: None

RESTRICTIONS:

A. Error Comments and Stops:

The program calls ENDJOB if

- a) $NFF > 1000$ where NFF is the number of values of a single wave function.
- b) $NF(JS(L)) < 6$ where $NF(JS(L))$ is the number of equidistant points in the r-range in which the forward and backward integrated solution of the Lth wave function are matched.

B. Range of Parameters:

- a) $NFF \leq 1000$ where NFF is the number of points of a single wave function.
- b) $JF \leq 20$ JF is the number of sets into which the r-range is divided. Each of these ranges is again subdivided into equal intervals.

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APPENDIX A

Listing of Program

```
FOR
C   MAIN HARTREE
COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
10 READ 1000,JF
20 READ 1001,(NF(J),XF(J),J=1,JF)
21 READ 1003,(JS(L),L=1,3)
22 DO 28 L=1,3
23 JSS=JS(L)
24 IF(6-NF(JSS))25,25,180
25 IS(L)=1+NF(JSS)/2
26 JS1=JSS-1
27 DO 28 J=1,JS1
28 IS(L)=IS(L)+NF(J)
30 NFF=1
40 DO 50 J=1,JF
50 NFF=NFF+NF(J)
60 IF(NFF-1000) 70,70,180
70 READ 1002,TE,TT,E(1),E(2),E(3),((P(L,N),L=1,3),N=1,NFF)
80 CALL RADIUS
90 DO 120 L=1,3
100 CALL SSRL(L)
105 X= SQRTF(S(L,NFF))
110 DO 120 N=1,NFF
120 P(L,N)=P(L,N)/X
130 CALL TEST
140 CALL ZPI
150 DO 160 L=1,3
160 CALL EIGEN(L)
170 GO TO 90
1000 FORMAT (I3)
1001 FORMAT (I4,E14.6)
1002 FORMAT (5E14.6/(3E14.6))
1003 FORMAT (3I3)
180 CALL SYSTEM
END
```

```

      FOR
      SUBROUTINE BINT(L)
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
      1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
20  B=.000000001
30  W=DX(JF)**2/12.
40  C=(ZNL(L,NFF-1)+E(L))*DX(JF)**2
50  X=C/2.+SQRTF(C*(1.+C/2.))
60  PB(NFF)=B/(1.+X)
70  PB(NFF-1)=B
80  NA=NFF
90  JA=JF-JS(L)+1
100 DO 190 K=1,JA
110  J=JF+1-K
120  NF1=NF(J)-1
130 DO 150 M=1,NF1
140  N=NA-1-M
150  PB(N)=(PB(N+1)*(2.+W*(ZNL(L,N+1)+E(L))*10.
      1                                     )+PB(N+2)*(W*(ZNL(L,N+2)+E(
      2L))-1.))/(1.-W*(ZNL(L,N)+E(L)))
160  NA=NA-NF(J)
170  M=NA-1
180  W=DX(J-1)**2/12.
190  PB(M)=(PB(M+1)*(2.+W*(ZNL(L,M+1)+E(L))*10.
      1                                     )+YF(PB(M+1),DX(J-1),1)*(W*
      2(YF(ZNL(L,M+1),DX(J-1),3)+E(L))-1.))/(1.-W*(ZNL(L,M)+E(L)))
      RETURN
      END

```

```

      FOR
      SUBROUTINE EIGEN(L)
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
      IS(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
10  CALL FINT(L)
20  EL=E(L)
30  AL=P(L,NFF)
40  E(L)=EL+.001
50  CALL FINT(L)
60  IF(SIGNF(1.,AL)*P(L,NFF)) 70,70,110
70  EU=EL
80  AU=AL
90  GO TO 210
110 IF(P(L,NFF)) 120,280,130
120 IF(AL-P(L,NFF)) 20,20,140
130 IF(AL-P(L,NFF)) 140,20,20
140 E(L)=EL-.001
150 GO TO 50
160 EO=E(L)
170 E(L)=(AU*EL-AL*EU)/(AU-AL)
180 DE=ABSF(EO-E(L))
190 IF(DE-TE) 280,200,200
200 CALL FINT(L)
210 IF(P(L,NFF)) 220,280,250
220 AL=P(L,NFF)
230 EL=E(L)
240 GO TO 160
250 AU=P(L,NFF)
260 EU=E(L)
270 GO TO 160
280 CALL BINT(L)
290 ISS=IS(L)
300 X=P(L,ISS)/PB(ISS)
310 DO 320 N=ISS,NFF
320 P(L,N)=PB(N)*X
330 CALL SSRL(L)
340 W=SQRTE(S(L,NFF))
350 DO 360 N=1,NFF
360 P(L,N)=P(L,N)/W
370 CALL ZPI
380 CALL PRINT(L)
390 IF(ABSF(A-E(L))-TE) 420,400,400
400 A=E(L)
410 GO TO 10
420 RETURN
      END

```

```

      FOR
      SUBROUTINE FINT(L)
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
      1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
10  FIRSTF(X)=X**(B+1.)*(1.-X  **11./(1.+B)+X  **2/(6.+4.*B)*((2.-B)*
      1121.-V)-11./(18.*(1.+B*9.))*((1.+B)*121.-(2.+5.*B)*V)*X  **3)
20  B=FLOATF(L/3)
30  W=DX(1)**2/12.
40  V=4.*(RR(1,NFF)/S(1,NFF)+RR(2,NFF)/S(2,NFF)+3.*RR(3,NFF)/S(3,NFF)
      1)-2.*RR(L,NFF)/S(L,NFF)-E(L)
60  P(L,1)=0.
80  P(L,2)=FIRSTF(R(2))
100 P(L,3)=FIRSTF(R(3))
110 K=1
120 KA=3
130 DO 210 J=1,JF
140 M=K+KA
150 K=K+NF(J)
160 DO 170 N=M,K
170 P(L,N)=(P(L,N-1)*(2.+W*(ZNL(L,N-1)+E(L))*10.)+ P(L,N-2)*(W*(ZNL
      1(L,N-2)+E(L))-1.))/(1.-W*(ZNL(L,N)+E(L)))
180 IF(J-JF) 190,210,190
190 W=DX(J+1)**2/12.
200 P(L,K+1)=(P(L,K)*(2.+W*(ZNL(L,K)+E(L))*10.)+YB(P(L,K-3),DX(J),3)*
      1W*(YB(ZNL(L,K-3),DX(J),3)+E(L))-1.))/(1.-W*(ZNL(L,K+1)+E(L)))
210 KA=2
220 RETURN
      END

```

```

      FOR
      SUBROUTINE OUTPUT
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
      1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000)
10  READ 1000,D1,D2
20  PRINT1001,D1,D2,E(1),E(2),E(3),TE,TT,R(1),P(1,1),P(2,1),P(3,1),
      1Z(1),ZNL(1,1),ZNL(2,1),ZNL(3,1)
30  M=1
40  DO 70 J=1,JF
50  K=M+1
60  M=M+NF(J)
70  PRINT 1002,(R(N),P(1,N),P(2,N),P(3,N),Z(N),ZNL(1,N),ZNL(2,N),ZNL
      1(3,N),N=K,M)
90  CALL ENDJOB
1000 FORMAT (2A5)
1001 FORMAT (1H1,36X,47HWAVE FUNCTIONS FOR SODIUM ION BY HARTREE METHOD
      1//55X,2A5////17X,3HE1=E14.9,17X,3HE2=E14.9,17X,3HE3=E14.9/
      2          25H ACCURACY OF EIGENVALUE=E14.6,40X,26HACCURACY OF WA
      3VEFUNCTIONS=E14.6///3H R13X,6HP1S(R),8X,6HP2S(R),8X,6HP2P(R),8X,4
      4HZ(R),11X,6HZ1S(R),8X,6HZ2S(R),8X,6HZ2P(R)//8E14.6)
1002 FORMAT (1H / (8E14.6))
1003 FORMAT (3E14.6)
      END

```

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```
      FOR
      SUBROUTINE PRINT(L)
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
      1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
      10 PRINT 1000 ,(P(L,N),PB(N),N=1,NFF),E(L)
      20 RETURN
      1000 FORMAT (2E18.9)
      END
```

```

      FOR
      SUBROUTINE RADIUS
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
      1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000)
10  K=1
20  A=0.
30  R(1)=0.
40  DO 100 J=1,JF
50  M=K+1
60  K=K+NF(J)
70  A=XF(J)-A
80  DX(J)=A/FLOATF(NF(J))
      A=XF(J)
90  DO 100 N=M,K
100 R(N)=R(N-1)+DX(J)
110 RETURN
      END

```

```

      FOR
      SUBROUTINE RINT(U)
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
      1,X1
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
      1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
      2,U(1000),X1(1000)
      A=DX(1)/12.
      X1(1)=0.
      U(1)=0.
      U(2)=A*(8.*X1(2)-X1(3))
      K=1
      DO 30 J=1,JF
      M=K+2
      K=K+NF(J)
      DO 20 N=M,K
      B=-X1(N-2)
      C=8.*X1(N-1)
      D=5.*X1(N)
20  U(N)=U(N-1)+A*(B+C+D)
      IF(J-JF) 25,30,35
25  A=DX(J+1)/12.
      B=-YB(X1(K-3),DX(J),1)
      C=8.*X1(K)
      D=5.*X1(K+1)
      U(K+1)=U(K)+A*(B+C+D)
30  CONTINUE
35  RETURN
      END

```

```

      FOR
      SUBROUTINE SSRL(L)
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
      1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
10  R(1)=1.
30  S(L,1)=0.
31  A=DX(1)/12.
32  B=8.*P(L,2)**2
33  C=-P(L,3)**2
40  S(L,2)=A*(B+C)
50  RR(L,1)=0.
60  RR(L,2) = A*(B/R(2)+C/R(3))
70  K=1
80  DO 170 J=1,JF
90  M=K+2
100 K=K+NF(J)
110 DO 130 N=M,K
111 B=-P(L,N-2)**2
112 C=8.*P(L,N-1)**2
113 D=5.*P(L,N)**2
120 S(L,N)=S(L,N-1)+A*(B+C+D)
130 RR(L,N)=RR(L,N-1)+A*(B/R(N-2)+C/R(N-1)+D/R(N))
140 IF(J-JF) 141,170,190
141 A=DX(J+1) /12.
142 B=-YB(P(L,K-3),DX(J),3)**2
143 C=8.*P(L,K)**2
144 D=5.*P(L,K+1)**2
150 S(L,K+1)=S(L,K)+4*(B+C+D)
160 RR(L,K+1)=RR(L,K)+A*(B/R(K-1)+C/R(K)+D/R(K+1))
170 CONTINUE
180 R(1)=0.
190 RETURN
      END

```

```

      FOR
      SUBROUTINE TEST
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
      IS(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
10  K=1
20  T=0.
30  DO 100 J=1,JF
40  M=K+2
50  K=K+NF(J)
60  A=0.
70  DO 80 N=M,K,2
80  A=A+SQ (N-2)+4.*SQ (N-1)+SQ (N)
90  A=A+FLOATF(NF(J)-(NF(J)/2)*2)*(-SQ (K-2)+8.*SQ (K-1)+5.*SQ (K))
      1/4.
100 T=T+A*DX(J)/3.
110 IF(T-TT) 120,120,130
120 CALL OUTPUT
130 DO 150 L=1,3
140 DO 150 N=1,NFF
150 PF(L,N)=(P(L,N)+PF(L,N))/2.
160 RETURN
      END

```

```

      FOR
      FUNCTION YB(A,D,L)
      DIMENSION A(10),D(2)
10  B=-D(2)
20  B1= B + D(1)
30  B2 = B1 + D(1)
40  B3 = B2 + D(1)
50  C=6.*D(1)**3
60  YB=(B1*B2*(A(3*L+1)*B3-A(1)*B)+3.*B*B3*(A(L+1)*B1-A(2*L+1)*B2))/C
70  RETURN
      END

```

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```
      FOR  
      FUNCTION YF(A,D,L)  
      DIMENSION A(7),D(2)  
10  B=A(2*L+1)-2.*A(L+1)+A(1)  
20  C=-A(2*L+1)+4.*A(L+1)-3.*A(1)  
30  X=D(1)/D(2)  
40  YF=(B*X+C)*X/2.+A(1)  
50  RETURN  
      END
```

```

SUBROUTINE YZ(P2)
COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
1,X1
DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
IS(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
2,P2(1000),X1(1000),U(1000)
DO 10 N=2,NFF
10 X1(N)=(P(3,N)*R(N))**2
CALL RINT(U)
DO 20 N=2,NFF
20 X1(N)=P(3,N)**2/R(N)**3
CALL RINT(P2)
P2(1)=0.
DO 30 N=2,NFF
H=R(N)**2
30 P2(N)=U(N)/H+H*R(N)*(P2(NFF)-P2(N))
RETURN
END

```

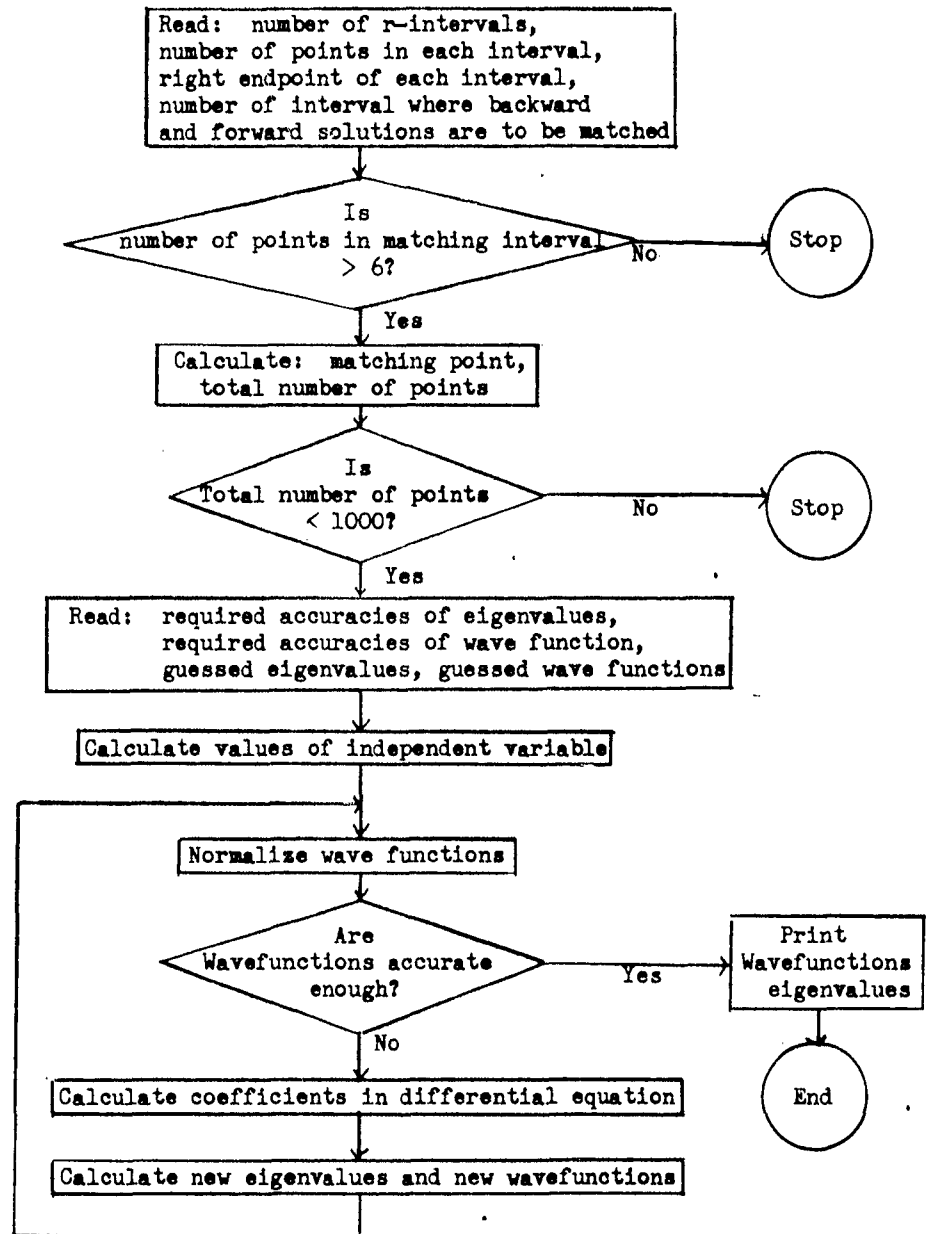
```

      FOR
      SUBROUTINE ZPI
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
      1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
10  R(1)=1.
      CALL Y2(Z)
30  DO 70 N=2,NFF
31  A=Y(1,N)
32  B=Y(2,N)
33  C=Y(3,N)
40  EE =-11.+2.*(A+B+3.*C)
41  D=2./R(N)
50  ZNL(1,N)=D*(EE -A)
60  ZNL(2,N)=D*(EE -B)
70  ZNL(3,N)=D*(EE -C-.4*Z (N)+1./R(N))
80  R(1)=0.
90  RETURN
      END

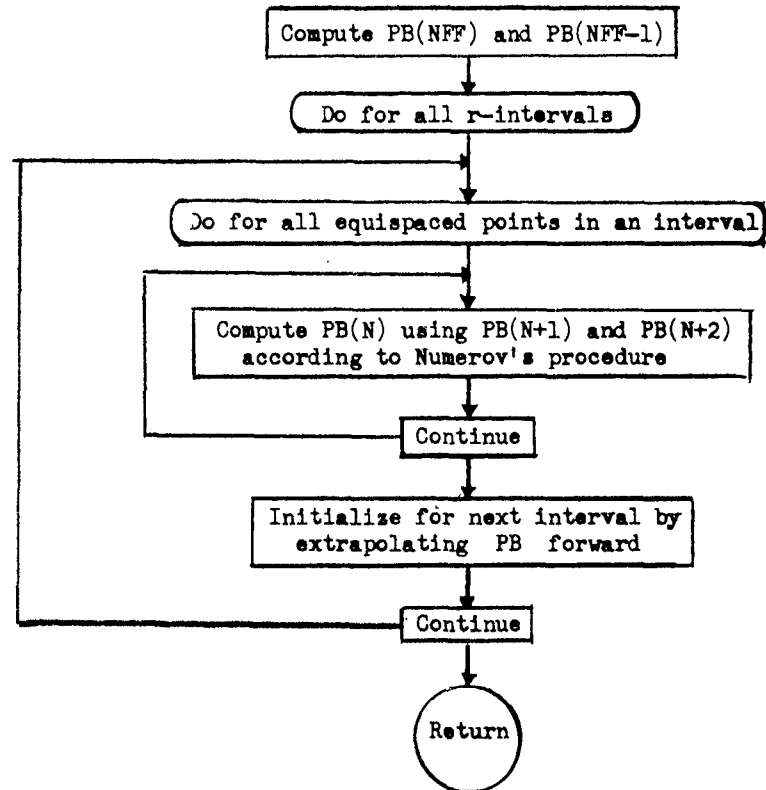
```

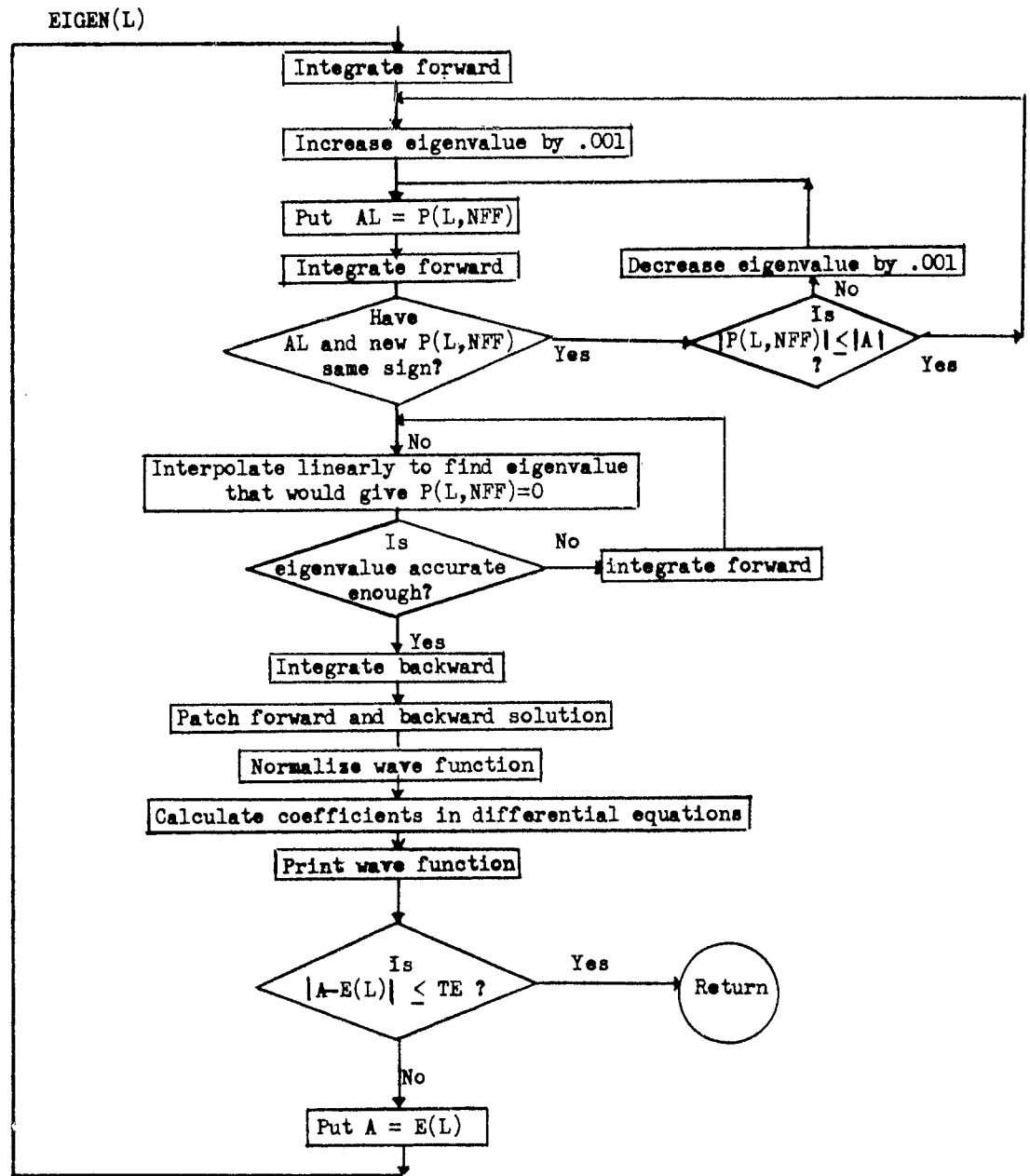
APPENDIX B - FLOW CHART

MAIN ROUTINE

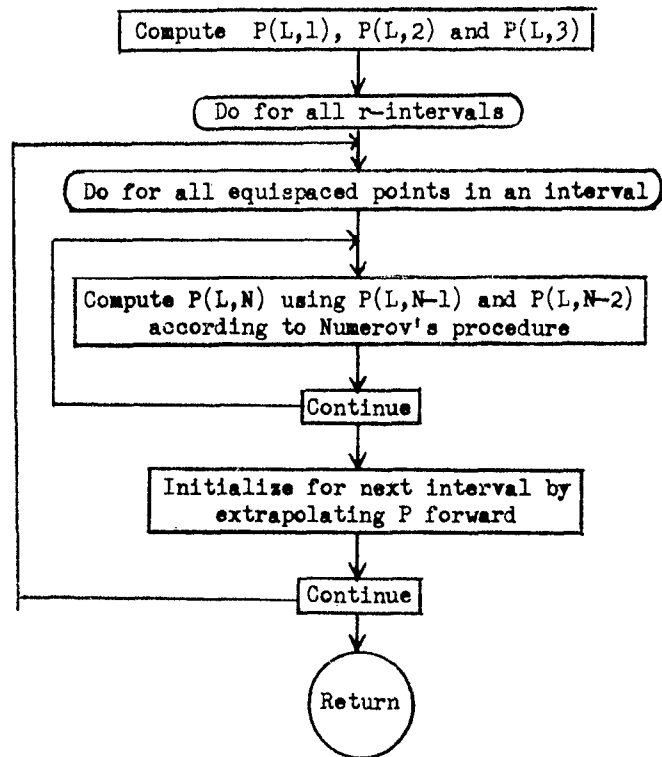


BINT(L)

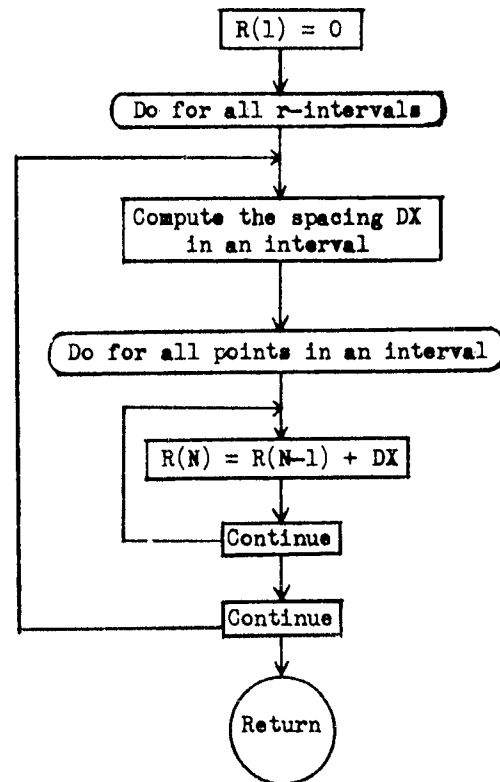




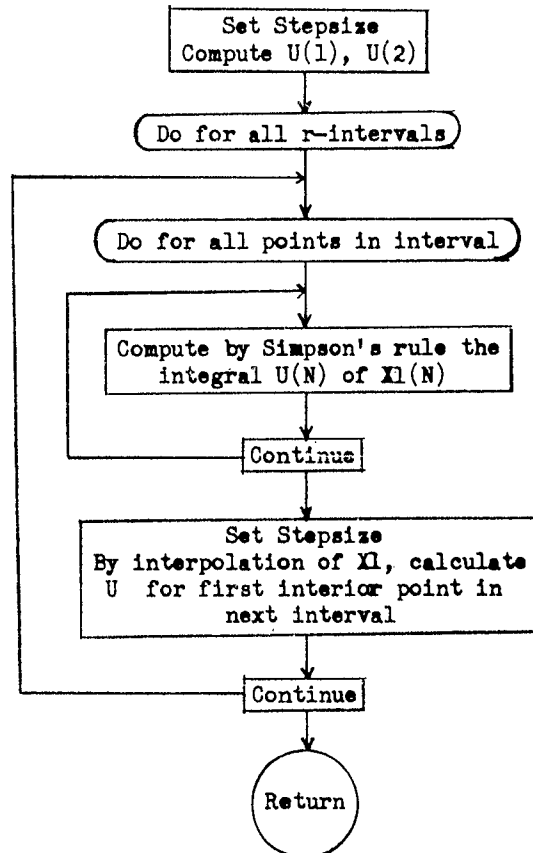
FINT(L)



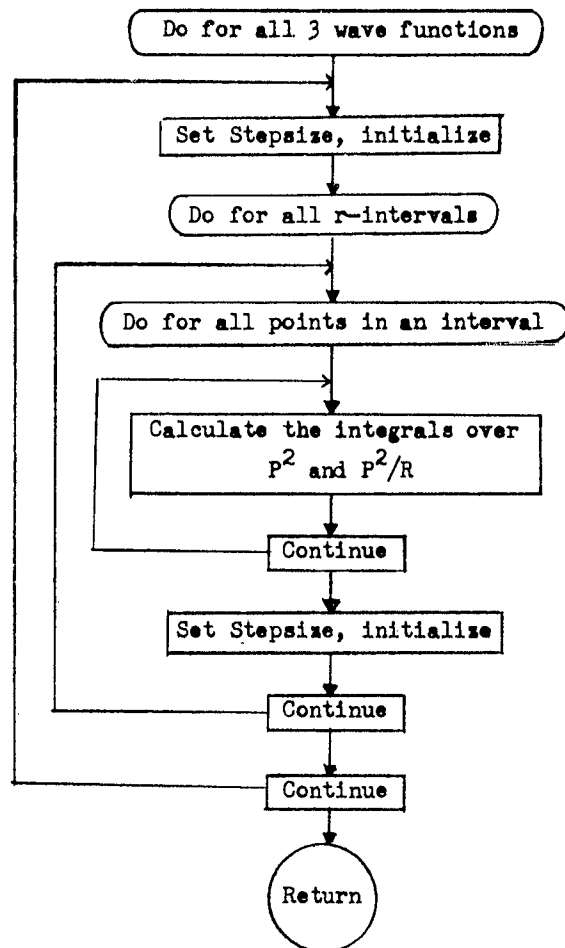
RADIUS



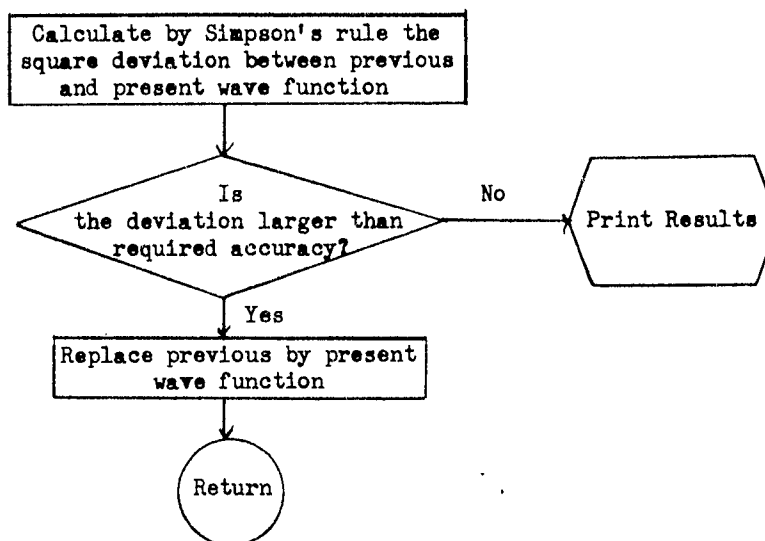
RINT(U)



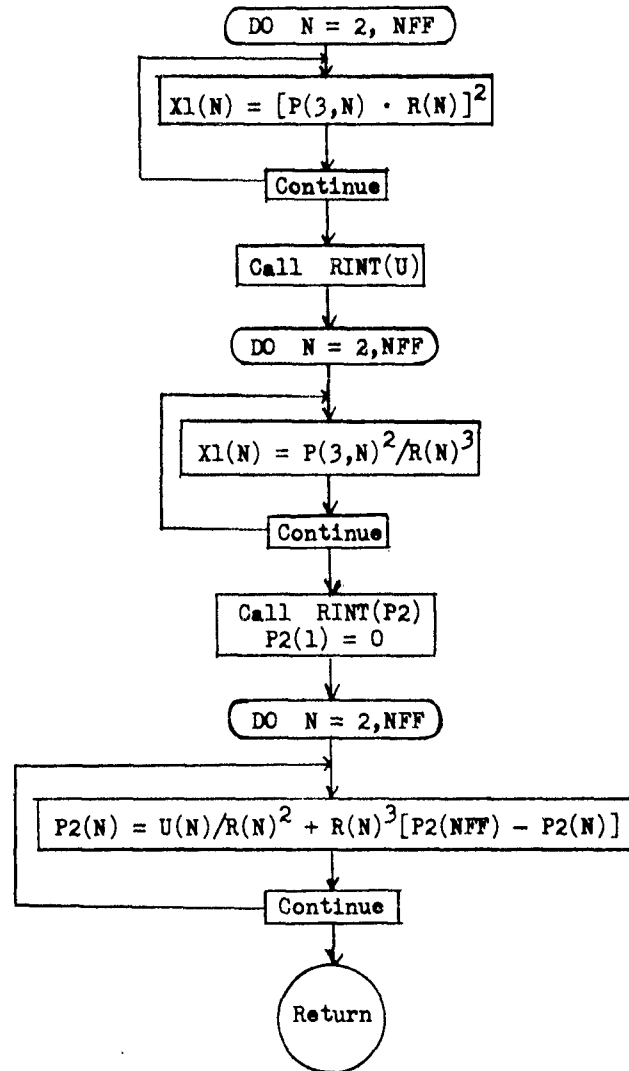
SSR



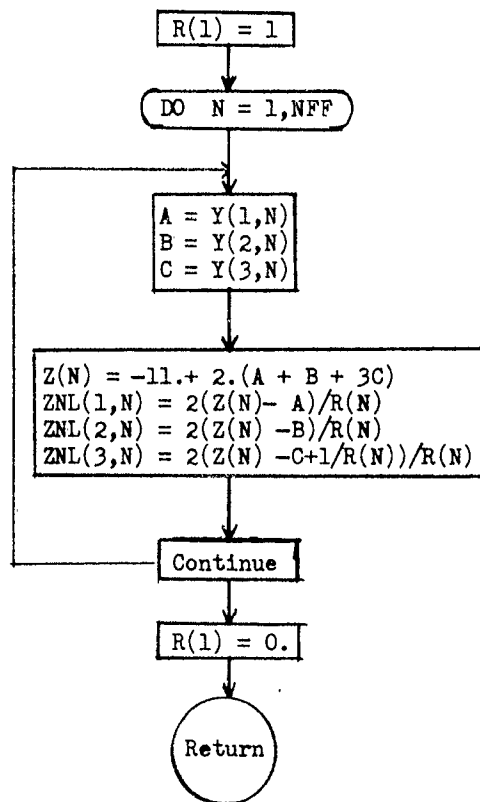
TEST



Y2(P2)



ZPI



APPENDIX C

EXAMPLE:

The r -range was chosen from 0 to 10.

It was divided into 5 sets, so $JF = 5$.

These sets were

from 0	to 0.04	0.01	so $NF(1) = 4$,	$XF(1) = .04$
0.04	0.2	0.02	$NF(2) = 8$,	$XF(2) = .2$
0.2	0.5	0.05	$NF(3) = 6$,	$XF(3) = .5$
0.5	1.2	0.1	$NF(4) = 7$,	$XF(4) = 1.2$
1.2	10	0.2	$NF(5) = 44$,	$XF(5) = 10$.

the forward and backward integrated solutions get matched in the interval

$$0.5 \leq r \leq 1.2 \quad \text{so}$$

$$JS(1) = 4 \quad JS(2) = 4 \quad JS(3) = 4$$

The permissible absolute error for the eigenvalues was chosen to be 10^{-4}

$$\text{so} \quad TE = 10^{-4}.$$

The permissible sum of squared deviations of wave functions was chosen to be 10^{-3}

$$\text{so} \quad TT = 10^{-3}.$$

The guesses for the 3 eigenvalues were taken as

$$E(1) = 81 \quad E(2) = 4.546948 \quad E(3) = 3.204463$$

Since $NFF = 1 + \sum_{j=1}^5 NF(J) = 70$ there follows three columns with 70 values

each for the guesses of the three wave functions.

The last input is the DATE 01-25-1962

EXAMPLE (INPUT)

NOLTR 63-31

TRA

5

4 .04

8 .2

6 .5

7 1.2

44 10.

4 4 4

.1

E-03

.1

E-02 81.

4.546948

3.204463

-0.	-0.	-0.
0.629350E 00	0.154058E-00	0.400036E-02
0.112863E 01	0.274103E-00	0.140013E-01
0.151784E 01	0.366138E-00	0.300027E-01
0.181501E 01	0.433163E-00	0.500045E-01
0.219322E 01	0.507191E 00	0.102009E-00
0.235731E 01	0.517195E 00	0.163015E-00
0.237832E 01	0.481181E-00	0.231021E-00
0.230628E 01	0.412155E-00	0.302027E-00
0.217621E 01	0.320121E-00	0.374034E-00
0.201312E 01	0.215081E-00	0.444040E-00
0.183502E 01	0.102038E-00	0.512046E 00
0.165292E 01	-0.150057E-01	0.578052E 00
0.122768E 01	-0.301114E-00	0.724065E 00
0.878488E 00	-0.555209E 00	0.842076E 00
0.614341E 00	-0.763288E 00	0.933084E 00
0.422235E-00	-0.923348E 00	0.997090E 00
0.287160E-00	-0.103739E 01	0.103909E 01
0.194108E-00	-0.111242E 01	0.106110E 01
0.880489E-01	-0.116944E 01	0.106110E 01
0.400222E-01	-0.113943E 01	0.102109E 01
0.180100E-01	-0.106140E 01	0.956086E 00
0.800445E-02	-0.958361E 00	0.880079E 00
0.300167E-02	-0.846319E 00	0.799072E 00
0.100056E-02	-0.736278E 00	0.718065E 00
-0.	-0.632238E 00	0.640058E 00
-0.	-0.455172E-00	0.501045E 00
-0.	-0.319120E-00	0.385035E-00
-0.	-0.220083E-00	0.292026E-00
-0.	-0.149056E-00	0.219020E-00
-0.	-0.101038E-00	0.163015E-00
-0.	-0.680257E-01	0.121011E-00
-0.	-0.450170E-01	0.890080E-01
-0.	-0.300113E-01	0.650058E-01
-0.	-0.200075E-01	0.480043E-01
-0.	-0.130049E-01	0.350031E-01
-0.	-0.900340E-02	0.260023E-01
-0.	-0.600226E-02	0.190017E-01
-0.	-0.400151E-02	0.140013E-01
-0.	-0.200075E-02	0.100009E-01
-0.	-0.914625E-03	0.691489E-02
0.	-0.120045E-02	0.488044E-02
-0.	-0.800305E-03	0.328030E-02
0.	-0.280106E-03	0.268024E-02
0.	-0.596273E-10	0.200018E-02
-0.	0.	0.148013E-02
0.	0.	0.120011E-02
-0.	-0.	0.800072E-03
0.	0.	0.280025E-03
0.	0.	0.119220E-09
0.	0.	0.

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-0.	-0.	-0.
0.	0.	0.
0.	0.	0.
-0.	-0.	-0.
0.	0.	0.
-0.	-0.	-0.
0.	0.	0.
0.	0.	0.
-0.	-0.	0.

01-25-1963

WAVE FUNCTIONS FOR SCATTERION BY PARTIAL METHOD

01-25-1962

EXAMPLE (OUTPUT)

E3=.32527596E 01
ACCURACY OF WAVEFUNCTIONS= 1.000000E-03E1=.18836413E 02
ACCURACY OF EIGENVALUES= 1.000000E-04

R	P1S(R)	P2S(R)	P2P(R)	Z(R)	Z1S(R)	Z2S(R)	Z2P(R)
J.	0.	0.	0.	0.	0.	0.	0.
0.00000E+00	0.639562E+00	0.150692E+00	0.352222E+02	0.150692E+00	-0.215144E+04	-0.213362E+04	0.178666E+05
0.20000E+01	0.114555E+01	0.267309E+00	0.132976E+01	0.127351E+03	-0.105192E+04	-0.103452E+04	0.396569E+04
0.30000E+01	0.153023E+01	0.356331E+00	0.263570E+01	0.424786E+03	-0.685591E+03	-0.669026E+03	0.155337E+04
0.40000E+01	0.182744E+01	0.4421653E+00	0.478404E+01	0.990840E+03	-0.503302E+03	-0.487071E+03	0.763061E+03
0.60000E+01	0.220334E+01	0.494053E+00	0.971976E+01	0.321302E+02	-0.321755E+03	-0.367046E+03	0.248532E+03
0.80000E+01	0.256337E+01	0.536233E+00	0.136467E+02	0.725342E+02	-0.231822E+03	-0.218592E+03	0.328227E+02
1.00000E+01	0.288427E+01	0.470884E+00	0.220184E+02	0.133731E+01	-0.173482E+03	-0.166665E+03	0.351424E+02
0.12000E+02	0.230905E+01	0.412486E+00	0.250470E+02	0.216866E+01	-0.173449E+03	-0.132842E+03	0.576103E+01
0.14000E+02	0.217736E+01	0.328768E+00	0.360223E+02	0.322185E+01	-0.118550E+03	-0.109221E+03	0.755209E+01
0.16000E+02	0.201231E+01	0.231170E+00	0.429372E+02	0.448173E+01	-0.100155E+03	-0.918781E+02	0.141983E+02
0.18000E+02	0.183549E+01	0.124404E+00	0.496707E+02	0.593046E+01	-0.859960E+02	-0.786477E+02	0.174267E+02
0.20000E+02	0.164712E+01	0.158450E+00	0.561277E+02	0.754371E+01	-0.747774E+02	-0.682472E+02	0.188658E+02
0.30000E+02	0.122020E+01	0.234643E+00	0.766347E+02	0.121177E+00	-0.549188E+02	-0.500484E+02	0.186907E+02
0.40000E+02	0.869475E+00	0.492213E+00	0.824612E+02	0.170974E+00	-0.417658E+02	-0.382903E+02	0.167398E+02
0.50000E+02	0.604112E+00	0.710673E+00	0.915252E+02	0.220982E+00	-0.329722E+02	-0.301619E+02	0.145258E+02
0.60000E+02	0.412280E+00	0.859067E+00	0.980926E+02	0.268222E+00	-0.264558E+02	-0.242994E+02	0.124786E+02
0.70000E+02	0.277697E+00	0.973689E+00	0.102245E+03	0.310697E+00	-0.215933E+02	-0.199306E+02	0.107098E+02
0.80000E+02	0.185228E+00	0.103536E+01	0.104598E+03	0.347223E+00	-0.178863E+02	-0.165997E+02	0.922459E+01
0.90000E+02	0.906478E+00	0.112668E+01	0.134830E+03	0.401843E+00	-0.127978E+02	-0.120155E+02	0.701710E+01
0.10000E+03	0.544718E+00	0.111537E+01	0.101163E+03	0.523422E+00	-0.957049E+01	-0.902035E+01	0.549981E+01
0.20000E+03	0.145029E+00	0.105482E+01	0.951252E+02	0.443334E+00	-0.745716E+01	-0.716278E+01	0.446410E+01
0.30000E+03	0.609100E+00	0.968093E+00	0.878930E+02	0.439473E+00	-0.602637E+01	-0.584437E+01	0.374489E+01
0.40000E+03	0.253533E+00	0.870342E+00	0.802032E+02	0.425243E+00	-0.502710E+01	-0.491412E+01	0.323378E+01
0.50000E+03	0.105396E+00	0.770689E+00	0.725174E+02	0.404301E+00	-0.430797E+01	-0.423750E+01	0.286065E+01
0.60000E+03	0.451309E+00	0.675220E+00	0.651039E+02	0.379422E+00	-0.377510E+01	-0.373111E+01	0.258021E+01
0.70000E+03	0.740344E+00	0.505907E+00	0.516722E+02	0.329955E+00	-0.305960E+01	-0.304121E+01	0.220013E+01
0.80000E+03	0.126685E+00	0.370480E+00	0.403755E+02	0.281385E+00	-0.259095E+01	-0.258359E+01	0.193778E+01
0.90000E+03	0.195765E+00	0.266977E+00	0.311857E+02	0.238547E+00	-0.226361E+01	-0.226063E+01	0.174644E+01
0.10000E+04	0.316485E+00	0.190087E+00	0.238699E+02	0.201997E+00	-0.201903E+01	-0.201784E+01	0.159706E+01
0.20000E+04	0.510225E+00	0.134069E+00	0.181350E+02	0.171679E+00	-0.182701E+01	-0.182653E+01	0.147491E+01
0.30000E+04	0.821181E+00	0.938365E+00	0.136921E+02	0.146793E+00	-0.167079E+01	-0.167060E+01	0.137188E+01
0.40000E+04	0.131713E+00	0.652597E+00	0.102823E+02	0.126423E+00	-0.154040E+01	-0.154032E+01	0.128315E+01
0.50000E+04	0.211935E+00	0.451409E+00	0.768568E+01	0.109717E+00	-0.142949E+01	-0.142946E+01	0.120559E+01
0.60000E+04	0.356989E+00	0.310796E+00	0.522133E+01	0.959470E+00	-0.133377E+01	-0.133376E+01	0.113706E+01
0.70000E+04	0.542498E+00	0.213120E+00	0.431370E+01	0.845193E+00	-0.125072E+01	-0.125020E+01	0.107599E+01
0.80000E+04	0.867339E+00	0.145623E+00	0.313702E+01	0.749615E+00	-0.117657E+01	-0.117657E+01	0.102118E+01
0.90000E+04	0.138559E+00	0.991899E+00	0.211232E+01	0.669095E+00	-0.111116E+01	-0.111116E+01	0.0971700E+00
0.10000E+05	0.221181E+00	0.673730E+00	0.169991E+01	0.600761E+00	-0.105266E+01	-0.105266E+01	0.0926795E+00
0.20000E+05	0.352332E+00	0.456468E+00	0.124668E+01	0.542390E+00	-0.100001E+01	-0.100001E+01	0.085858E+00
0.30000E+05	0.562504E+00	0.308565E+00	0.912234E+00	0.492043E+00	-0.952387E+00	-0.952387E+00	0.0848380E+00
0.40000E+05	0.896281E+00	0.208159E+00	0.662234E+00	0.448446E+00	-0.909094E+00	-0.909094E+00	0.0813942E+00
0.50000E+05	0.142740E+00	0.140135E+00	0.485682E+00	0.410360E+00	-0.869567E+00	-0.869567E+00	0.0782186E+00
0.60000E+05	0.227220E+00	0.942067E+00	0.355395E+00	0.376909E+00	-0.853355E+00	-0.853355E+00	0.0752811E+00

0.500000E 01	0.361448E-18	-0.432221E-03	0.256753E-02	0.347377E-01	-0.800001E 00	-0.800001E 00	-0.725559E 00
0.520000E 01	0.575065E-19	-0.423665E-03	0.186265E-02	0.321179E-01	-0.769231E 00	-0.769231E 00	-0.700208E 00
0.540000E 01	0.914349E-20	-0.283535E-03	0.134443E-02	0.297833E-01	-0.740741E 00	-0.740741E 00	-0.676566E 00
0.560000E 01	0.145332E-20	-0.189503E-03	0.976363E-03	0.276942E-01	-0.714286E 00	-0.714286E 00	-0.654467E 00
0.580000E 01	0.230928E-21	-0.126513E-03	0.705590E-03	0.258173E-01	-0.689655E 00	-0.689655E 00	-0.633763E 00
0.600000E 01	0.366332E-22	-0.843693E-04	0.509338E-03	0.241249E-01	-0.666667E 00	-0.666667E 00	-0.614328E 00
0.620000E 01	0.582360E-23	-0.562073E-04	0.367264E-03	0.225936E-01	-0.645161E 00	-0.645161E 00	-0.596048E 00
0.640000E 01	0.924919E-24	-0.374101E-04	0.264385E-03	0.212036E-01	-0.625000E 00	-0.625000E 00	-0.578822E 00
0.660000E 01	0.146813E-24	-0.248770E-04	0.190444E-03	0.192380E-01	-0.606061E 00	-0.606061E 00	-0.562564E 00
0.680000E 01	0.232495E-25	-0.165289E-04	0.136929E-03	0.187824E-01	-0.588235E 00	-0.588235E 00	-0.547192E 00
0.700000E 01	0.369637E-26	-0.107735E-04	0.983795E-04	0.177245E-01	-0.571429E 00	-0.571429E 00	-0.532638E 00
0.720000E 01	0.586388E-27	-0.727988E-05	0.706269E-04	0.167535E-01	-0.555556E 00	-0.555556E 00	-0.518937E 00
0.740000E 01	0.936613E-28	-0.482616E-05	0.506651E-04	0.158601E-01	-0.540541E 00	-0.540541E 00	-0.505752E 00
0.760000E 01	0.147474E-28	-0.319727E-05	0.363173E-04	0.150363E-01	-0.526316E 00	-0.526316E 00	-0.493273E 00
0.780000E 01	0.233614E-29	-0.211684E-05	0.260178E-04	0.142751E-01	-0.512821E 00	-0.512821E 00	-0.481412E 00
0.800000E 01	0.370642E-30	-0.140066E-05	0.186261E-04	0.135793E-01	-0.500000E 00	-0.500000E 00	-0.470107E 00
0.820000E 01	0.587433E-31	-0.926260E-06	0.133262E-04	0.129164E-01	-0.487805E 00	-0.487805E 00	-0.459321E 00
0.840000E 01	0.930735E-32	-0.612203E-06	0.952870E-05	0.123087E-01	-0.476191E 00	-0.476191E 00	-0.449018E 00
0.860000E 01	0.147311E-32	-0.404416E-06	0.660949E-05	0.117428E-01	-0.465116E 00	-0.465116E 00	-0.439167E 00
0.880000E 01	0.233702E-33	-0.267023E-06	0.486361E-05	0.112151E-01	-0.454545E 00	-0.454545E 00	-0.429739E 00
0.900000E 01	0.376209E-34	-0.176219E-06	0.347193E-05	0.107222E-01	-0.444444E 00	-0.444444E 00	-0.420706E 00
0.920000E 01	0.566360E-35	-0.116230E-06	0.247718E-05	0.102611E-01	-0.434783E 00	-0.434783E 00	-0.412045E 00
0.940000E 01	0.928871E-36	-0.766303E-07	0.176648E-05	0.982910E-02	-0.425532E 00	-0.425532E 00	-0.403734E 00
0.960000E 01	0.147673E-36	-0.504871E-07	0.125896E-05	0.942382E-02	-0.416667E 00	-0.416667E 00	-0.395751E 00
0.980000E 01	0.332321E-07	-0.332321E-07	0.896650E-06	0.904310E-02	-0.408163E 00	-0.408163E 00	-0.388077E 00
1.000000E 01	0.	-0.218393E-07	0.638039E-06	0.866505E-02	-0.400000E 00	-0.400000E 00	-0.380695E 00

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