Table 3. FORTRAN program for calculation of the large-*D* expansion for “frozen planetary” states of two-electron atoms

File c:\sergeev\ou\fortran\helium\summat\table3.txt
and also files: c:\sergeev\ou\fortran\helium\largen32*.f

```
      PROGRAM LARGE N 32
       implicit complex*32(a-h,o-z)
       DIMENSION EN(25),RA1(25),
      -   WFUN(300
     .          000),VX(75,75,75),AL(3),ZZ(3),SCR(3),X(3
     .          ),
      -   param(10),ee(40,20),om(3)
       EQUIVALENCE
     .          (PARAM(1),ZZ(1)),(PARAM(4),SCR(1)),(PARA
     .          M(7),DNU)
       character*11 name
   99  ifun=1
       ipri=0
       isym=0
c      PRINT*,'Enter NCOEF, RNOR (3 for 1/D, 2 for
     .          1/(D-1))'
c      PRINT*,'Enter NCOEF'
c      READ*,NCOEF,irnor
       READ*,NCOEF,iz
       if(ncoef.eq.0)stop
       name=' '
       if(iz.eq.2)name='He (Z=2)'
       if(iz.eq.3)name='Li+ (Z=3)'
c      rnor=irnor
   20  format(1x,a8,i4,6f11.6)
c      PRINT*,'DNU,RNOR = '
c      READ*,DNU,RNOR
       dnu=1
c      PRINT*,'Enter IPA1,IPA2,IPA3'
c      READ*,IPA1,IPA2,IPA3
c      print*,'Enter n1'
       read*,n1,n2,n3
       ipa1=n3+1
       ipa2=n1+1
       ipa3=n2+1
       irnor=2*ipa2
       rnor=irnor
c      PRINT20,'NCOEF =',ncoef
       print100,name,n1,n2,n3
  100  format(1x,a11,
     .   ' asymmetric-configuration state
     .          (',i2,',',i2,',',
     .    i2,')')
       write(1,*)n1,n2,n3,ncoef,irnor-3,name
c      PRINT*,IPA1,IPA2,IPA3
c      PRINT*,'AL = '
c      READ*,AL
       al(1)=1
       al(2)=1
       al(3)=0
c      PRINT40,'1/m1, 1/m2, 1/m3 =',(real(al(i)),i=1,3)
c      PRINT*,'ZZ = '
c      READ*,ZZ
       zz(1)=-iz
       zz(2)=-iz
       zz(3)=1
c      PRINT40,'Z2*Z3, Z3*Z1, Z1*Z2
     .          =',(real(zz(i)),i=1,3)
c      PRINT*,('-',I=1,100),' SCR = '
c      READ*,SCR(1),SCR(2),SCR(3)
       scr(1)=0
       scr(2)=0
       scr(3)=0
c      PRINT*,SCR
c      r1=1.d-2
c      r2=1.d-2
c      r3=1.d-2
       if(iz.ne.2)goto302
       r1=(.12q0,-.35q0)/2
       r2=.19q0/2
       r3=(.15q0,-.24q0)/2
       om(1)=(14.66q0,-4.18q0)*2
       om(2)=(11.79q0,5.74q0)*2
       om(3)=(2.26q0,4.28q0)*2
       goto301
  302  if(iz.ne.3)goto303
       r1=(.05q0,-.32q0)/iz
       r2=(.16q0,-.02q0)/iz
       r3=(.08q0,-.19q0)/iz
       om(1)=sqrt((411.0q0,-105.5q0))*iz**2/2
       om(2)=sqrt((35.7q0,267.7q0))*iz**2/2
       om(3)=sqrt((-56.4q0,23.5q0))*iz**2/2
       goto301
  303  print*,'Z!!!'
       stop
  301  x(1)=r1**2
       x(2)=r2**2
       x(3)=r3**2
       LPB=ISYM
       CALL TBNEXP(AL,IFUN,PARAM,RNOR,IPA1,IPA2,IPA3,
      -   NCOEF,EN,om,IPRI,X,WFUN,300 000,VX,75,LPB)
       PRINT10,'r1,2,3 = ',(sqrt(x(n)),n=1,3)
   10  format(1x,a11,3(2x,2f10.6))
   40  format(1x,a44,3f11.6)
   50  format(10(2x,2f8.5))
   60  format(1x,a11,3(2x,2f10.6)/(12x,3(2x,2f10.6)))
       PRINT10,'Omega = ',om
c      PRINT30,'En-coeff.=',(EN(I),I=1,NCOEF)
       write(1,*)(en(i),i=1,ncoef)
   30  FORMAT(1x,a10,2(2x,2d16.8)/(11x,2(2x,2d16.8)))
       ndim=3
       D=NDIM-3+RNOR
       C=1/D
       ndim1=5
       D1=NDIM1-3+RNOR
       C1=1/D1
c      PRINT60,'En-Pade
     .          =',(c**2*padesum(en,c,i),I=1,NCOEF)
       d=c**2
       print80
   80  format(2x,'n',7x,'Coefficients of 1/N-
     .          expansion',12x,
     .    'Padé approximants',12x,'Padé (D = 5)')
       do 1 n=1,ncoef
    1  print70,n-
     .          1,en(n),c**2*padesum(en,c,n),c1**2*pades
     .          um(en,c1,n)
   70  format(i3,2d20.12,2(3x,2f12.8))
       print130
  130  format('    Partial sums:  Shanks transform:
     .          Second Shanks:',
     .    '     Third Shanks:    Fourth Shanks:')
       RA1(1)=D*EN(1)
       DO201I=2,NCOEF
       a=1-1
  201  RA1(I)=RA1(I-1)+C**a*EN(I)*D
       DO 11 N=1,NCOEF
   11  EE(N,1)=RA1(N)
       MM=(NCOEF+1)/2
       DO 12 M=2,MM
       N1=NCOEF-M+1
       DO 12 N=M,N1
   12  EE(N,M)=(EE(N+1,M-1)*EE(N-1,M-1)-EE(N,M-1)**2)
      -  /(EE(N+1,M-1)+EE(N-1,M-1)-EE(N,M-1)*2)
       DO 13 N=1,NCOEF
       MM=MIN0(N,NCOEF-N+1)
   13  PRINT59,(EE(N,M),M=1,MM)
       PRINT120,LPB
  120  format(48x,i6,' components of wave function'/)
       m=101
       do 2 n=1,m
       cn=(n-1)*2*c/(m-1)
       c1=cn/2
    2  write(2,90)real(cn),(padesum(en,c1,i)/4,i=ncoef-
     .          2,ncoef)
   90  format(f9.4,10(',',f10.5))
       goto99
       END
       SUBROUTINE
     .          TBNEXP(AL,IFUN,PARAM,RNOR,IPA1,IPA2,IPA3
     .          ,
     .    NCOEF,EN,om,IPRINT,X,WFUN,MWFUN,VX,MVX,LPB)
       implicit complex*32(a-h,o-z)
       DIMENSION AL(3),PARAM(10),X(3),S1(3),F(3,4),
      -IND(6),EN(25),DI(3),A2(6,6),H3(3,3,3),EVR(6),
      -
     .          EVI(6),AE(6,6),AAA(6,6),OM(3),AH3(6,6,6)
     .          ,V(99),
     .    IK(3),LCH(99),KPB(3),IKL(3),
      -WFUN(MWFUN),VX(MVX,MVX,MVX)
      -   ,AM(3,3),BM(3,3)
      -   ,VEX(3,99),BE(3),V1(99),V2(99),pol(4)
c     . rrep(9),rimp(9),rrez(9),rimz(9)
c     . rrea(3,3),rima(3,3),rrez(9),rimz(9)
c      real*8 rrep,rimp,rrez,rimz,rr0,rr1,rtol,x02aaf
       real*16 rr0,rr1
       LOGICAL LO
       rr0=0
       rr1=1
       ci=cmplx(rr0,rr1)
c      IPR=(IPRINT-1)*(100-IPRINT)
       ipri=iprint
       ISYM=LPB+1
    1  FORMAT(2X,A6,2X,3D10.2,10X,3D10.2)
       IF(IPRI.GT.0)PRINT*,'PARAM=',PARAM,',
     .          RNOR=',RNOR
   80  FORMAT(4I3)
C           MiHiMizAcia gAMil'TOHiAHA
       D=0
       DO3N=1,200
       CALL TAYLOR(X,VEX,3,V,V1,V2,IFUN,PARAM)
       S1(1)=X(2)+X(3)-X(1)
       S1(2)=X(1)+X(3)-X(2)
       S1(3)=X(1)+X(2)-X(3)
       S=X(1)*X(2)+X(2)*X(3)+X(3)*X(1)-X(1)**2/2
      -   -X(2)**2/2-X(3)**2/2
       R=AL(1)*X(1)+AL(2)*X(2)+AL(3)*X(3)
       DO202I=1,3
       F(I,4)=(AL(I)/S-R*S1(I)/S**2)/4+VEX(I,2)
       DO202K=1,3
       A=1
       B=0
       IF(I.NE.K)GOTO2
       A=-1
       B=VEX(I,3)*2
    2  F(I,K)=(2*R*S1(I)*S1(K)/S**3-(R*A
      -   +AL(I)*S1(K)+AL(K)*S1(I))/S**2)/4+B
  202  BM(I,K)=F(I,K)/2
       CALL MATIN2(F,3,3,4,1,IND,I,A)
       D1=F(1,4)**2+F(2,4)**2+F(3,4)**2
       IF(abs(D1).GE.abs(D).AND.abs(D1/(X(1)**2+X(2)**2
      -   +X(3)**2)).LT.1.D-8)GOTO10
       D=D1
       DO4I=1,3
    4  X(I)=X(I)-F(I,4)
    5  FORMAT(A7,I5,5D25.18)
       IF(N.LT.10.AND.IPRI.GT.0)PRINT5,' N,X,D',N,X,D
    3  CONTINUE
   10  EN(1)=R/S/4
      -   +VEX(1,1)+VEX(2,1)+VEX(3,1)
       IF(IPRI.GT.0)PRINT5,' NXD,EN',N,X,D,EN(1)
       IF(NCOEF.EQ.1)RETURN
       DO11I=1,3
   11  DI(I)=-S1(I)/S/4
       IF(IPRI.GT.0)PRINT30,' DI',DI
C           HAXOzdEHiE KOef. KB. fOPMy
       DO12I=1,3
       DO12K=1,3
       IF(I.EQ.K)GOTO12
       L=6-I-K
       IF(I.LT.K)GOTO14
       C=AL(I)+AL(K)
       BE(L)=C
       A2(L+3,L)=2*C*X(L)
       A2(L+3,L+3)=2*C*DI(L)+AL(I)*DI(K)+AL(K)*DI(I)
       A2(L,L)=-A2(L+3,L+3)
       A2(L,L+3)=VEX(L,3)
       H3(L,L,L)=-2*C
       AM(L,L)=-C*2*X(L)
   14  A2(I+3,K)=AL(L)*S1(L)
       A2(I+3,K+3)=-AL(K)*DI(L)+AL(L)*DI(K)
       A2(K,I)=-A2(I+3,K+3)
       A2(I,K+3)=0
       H3(I,L,K)=AL(L)
       H3(I,I,K)=-AL(L)
       H3(I,K,K)=-AL(L)
       H3(I,K,I)=0
       AM(I,K)=-AL(L)*S1(L)
   12  CONTINUE
   13  FORMAT(/(3D20.10,6X,3D20.10))
C           diAgOHAlizAcia KB. fOPMy
  199  FORMAT(2D40.23)
       DO131 I=1,3
        DO 131 K=1,3
       AE(I,K)=0
       DO 131 L=1,3
  131  AE(I,K)=AE(I,K)+AM(L,I)*BM(L,K)
       pol(1)=-1
       pol(2)=ae(1,1)+ae(2,2)+ae(3,3)
       pol(3)=-(ae(2,2)*ae(3,3)-ae(2,3)*ae(3,2)+
      . ae(1,1)*ae(3,3)-ae(1,3)*ae(3,1)+ae(1,1)*ae(2,2)-
     .          ae(1,2)*ae(2,1))

     .          pol(4)=ae(1,1)*ae(2,2)*ae(3,3)+ae(1,2)*a
     .          e(2,3)*ae(3,1)+
      . ae(1,3)*ae(2,1)*ae(3,2)-ae(1,1)*ae(2,3)*ae(3,2)-
      . ae(1,2)*ae(2,1)*ae(3,3)-ae(1,3)*ae(2,2)*ae(3,1)
c      rrep(1)=pol(1)
c      rrep(2)=pol(2)
c      rrep(3)=pol(3)
c      rrep(4)=pol(4)
c      rimp(1)=pol(1)*(-ci)
c      rimp(2)=pol(2)*(-ci)
c      rimp(3)=pol(3)*(-ci)
c      rimp(4)=pol(4)*(-ci)
       do 502 nom=1,3
       d=0
       xom=-om(nom)**2
       do 501 n=1,200

     .          d1=(pol(1)*xom**3+pol(2)*xom**2+pol(3)*x
     .          om+pol(4))/
      . (3*pol(1)*xom**2+2*pol(2)*xom+pol(3))
       if(abs(d1).ge.abs(d) .and. abs(d1/xom).lt.1.d-
     .          8)goto509
       d=d1
c      if(n.lt.5.and.nom.eq.1)print*,'n,xom,d',n,xom,d
       xom=xom-d
  501  continue
  509  if(n.gt.100)print*,'OMEGA no found: nom, iter,
     .          d',nom,n,d
  502  om(nom)=sqrt(-xom)
c      n=4
c      rtol=x02aaf(rtol)
c      ifail=0
c      call C02ADF(rrep,rimp,n,rrez,rimz,rtol,ifail)
c      if(n.ne.1)print*,'C02ADF failed to find
     .          frequences, n =',n
c
c      do 782 i=1,3
c      do 782 k=1,3
c      rrea(i,k)=ae(i,k)
c 782  rima(i,k)=-ae(i,k)*ci
c      ifail=0
c      call F02AJF(rrea,3,rima,3,3,rrez,rimz,ind,ifail)
c      if(ifail.ne.0)print*,'F02AJF failed to find
     .          eigenvalues'
       DO 784 I=1,3
c      c=cmplx(rrez(i),rimz(i))
c  784 EVR(I)=SQRT(-c)
  784  EVR(I)=om(i)
       DO 132 I=1,3
  132  EVR(I+3)=-EVR(I)
       DO 133 L=1,6
       AE(1,L)=1
       DO 134 I=1,5
       DO 135 K=1,5
  135  AAA(I,K)=A2(I+1,K+1)
       AAA(I,I)=AAA(I,I)-EVR(L)
  134  AAA(I,6)=-A2(I+1,1)
       CALL MATIN2(AAA,6,5,6,1,IND,NE,D)
       DO 133 I=1,5
  133  AE(I+1,L)=AAA(I,6)
       DO21K=1,6
       EVI(K)=-1.D18
       DO21K1=1,6
       IF(real(EVR(K1)).LT.real(EVI(K)))GOTO21
       IF(K.EQ.1)GOTO22
       K9=K-1
       DO23K2=1,K9
       IF(IND(K2).EQ.K1)GOTO21
   23  CONTINUE
   22  EVI(K)=EVR(K1)
       IND(K)=K1
       DO24I=1,6
   24  AAA(I,K)=AE(I,K1)
   21  CONTINUE
       DO25I=1,3
   25  OM(I)=-EVI(I+3)
       DO26I=1,6
       A=AAA(I,1)
       AA(I,1)=AAA(I,3)
   26  AAA(I,3)=A
       IF(IPRI.GT.0)PRINT30,' EVI,OM',EVI,OM
       DO15K=1,3
       C=0
       DO16I=1,3
   16  C=C+AAA(I,K)*AAA(I+3,K+3)-AAA(I+3,K)*AAA(I,K+3)
       DO15I=1,6
   15  AAA(I,K+3)=AAA(I,K+3)/C
       IF(IPRI.GT.0)PRINT5,' AAA'
       IF(IPRI.GT.0)PRINT13,((AAA(I,K),K=1,6),I=1,6)
C
       N=2*NCOEF-1
       CALL TAYLOR(X,VEX,N,V,V1,V2,IFUN,PARAM)
       DO 301 M9=1,N
       M=N-M9+1
       IF(abs(VEX(1,M)).NE.0.OR.abs(VEX(2,M)).NE.0.OR.
      -   abs(VEX(3,M)).NE.0)GOTO302
  301  CONTINUE
  302  MVEX=M
       DO17I1=1,6
       DO17K1=1,6
       DO17L1=1,6
       C=0
       DO18I=1,3
       DO18K=1,3
       DO18L=1,3
       IF(I.EQ.K.AND.K.EQ.L)C=C +
     .          AAA(I+3,I1)*AAA(K+3,K1)
      -   *AAA(L+3,L1)*VEX(I,4)
   18  C=C+AAA(I,I1)*AAA(K+3,K1)*AAA(L,L1)*H3(I,K,L)
   17  AH3(I1,K1,L1)=C
       DO 19 I1=1,6
       DO 19 I=1,3
       C=RNOR*BE(I)*AAA(I,I1)
       AH3(I1,1,4)=AH3(I1,1,4)+C
   19  AH3(I1,4,1)=AH3(I1,4,1)-C
   98  FORMAT(A7,5D24.16/7X,(5D24.16))
       IF(IPRI.GT.0)PRINT80,IPA1,IPA2,IPA3,NCOEF
       NM=NCOEF-2
       NMD=NM*2
       NMD2=NMD+2
   30  FORMAT(A6,(10D12.4))
       EN(2)=(2*IPA1-1)*OM(1)+(2*IPA2-1)*OM(2)+(2*IPA3-
     .          1)*OM(3)
      -   +RNOR*(BE(1)*DI(1)+BE(2)*DI(2)+BE(3)*DI(3))
       IF(IPRI.GT.0)PRINT5,' EN(2)',2,EN(2)
       IF(NCOEF.EQ.2)RETURN
C           BycICLEHiE pOpPABOK TB
       KPA1=MIN0(3*NM+1,IPA1)
       KPA2=MIN0(3*NM+1,IPA2)
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```
      KPA3=MIN0(3*NM+1,IPA3)
      KPAS=KPA1+KPA2+KPA3
      KM1=KPA1+3*NM
      KM2=KPA2+3*NM
      KM3=KPA3+3*NM
      IK1=IPA1-KPA1
      IK2=IPA2-KPA2
      IK3=IPA3-KPA3
      IK(1)=IK1
      IK(2)=IK2
      IK(3)=IK3
      WFUN(1)=1
      LCH(1)=0
      LCH(2)=1
      LPB=1
      DO100NFB=1,NMD
  200 FORMAT(' NFB,CT,RT',I5,2F20.5)
      MDIB1=MIN0(3*NFB,3*(NMD-NFB))
      MAXB1=KPA1+MDIB1
      MINB1=MAX0(KPA1-MDIB1,1)
      DO51KPB1=MINB1,MAXB1
      MDIB2=MDIB1-IABS(KPB1-KPA1)
      MAXB2=KPA2+MDIB2
      MINB2=MAX0(KPA2-MDIB2,1)
      DO51KPB2=MINB2,MAXB2
      MDIB3=MDIB2-IABS(KPB2-KPA2)
      MAXB3=KPA3+MDIB3
      IN=1
      IS=KPAS+KPB1+KPB2+NFB
      IF(IS/2*2.EQ.IS)IN=2
      MINB3=MAX0(KPA3-MDIB3,IN)
      DO51KPB3=MINB3,MAXB3,2
      A=0
      LPB=LPB+1
      GOTO(310,311,312,313),ISYM
  311 K=KPB1-KPA1
      GOTO314
  312 K=KPB2-KPA2
      GOTO314
  313 K=KPB3-KPA3
  314 IF((K/2)*2.NE.K)GOTO62
  310 KPBS=KPB1+KPB2+KPB3
C           CYMMiPOBAHiE KYbic. cl.
      DO36K1=1,KM1
      DO36K2=1,KM2
      DO36K3=1,KM3
   36 VX(K1,K2,K3)=0
      DO32I=1,6
      DO32K=1,6
      DO32L=1,6
      KPB(1)=KPB1
      KPB(2)=KPB2
      KPB(3)=KPB3
      IKL(1)=L
      IKL(2)=K
      IKL(3)=I
      B=1
      DO33M=1,3
      IL=IKL(M)
      IF(IL.GT.3)GOTO34
      KPB(IL)=KPB(IL)-1
      B=B*(KPB(IL)+IK(IL))
      GOTO33
   34 IL=IL-3
      KPB(IL)=KPB(IL)+1
   33 CONTINUE
      KB1=KPB(1)
      KB2=KPB(2)
      KB3=KPB(3)

               IF(KB1.GT.0.AND.KB1.LE.KM1.AND.KB2.GT.0.
               AND.KB2.LE.KM2
     -.AND.KB3.GT.0.AND.KB3.LE.KM3)
     -   VX(KB1,KB2,KB3)=VX(KB1,KB2,KB3)-B*AH3(I,K,L)
   32 CONTINUE
      LPC=LCH(NFB)
      MDIC1=MIN0(3*(NFB-1),3*(NMD-NFB+1))
      MAXC1=KPA1+MDIC1
      MINC1=MAX0(KPA1-MDIC1,1)
      MDBC1=3
      DO82KPC1=MINC1,MAXC1
      MDIC2=MDIC1-IABS(KPC1-KPA1)
      MAXC2=KPA2+MDIC2
      MINC2=MAX0(KPA2-MDIC2,1)
      MDBC2=MDBC1-IABS(KPC1-KPB1)
      DO82KPC2=MINC2,MAXC2
      MDIC3=MDIC2-IABS(KPC2-KPA2)
      MAXC3=KPA3+MDIC3
      IN=1
      IS=KPAS+KPC1+KPC2+NFB-1
      IF(IS/2*2.EQ.IS)IN=2
      MINC3=MAX0(KPA3-MDIC3,IN)
      MDBC3=MDBC2-IABS(KPC2-KPB2)
      DO82KPC3=MINC3,MAXC3,2
      LPC=LPC+1
      IF(MDBC3-IABS(KPC3-KPB3).GE.0)
     -   A=A+VX(KPC1,KPC2,KPC3)*WFUN(LPC)
   82 CONTINUE
C
      IF(NFB.EQ.1)GOTO63
      IF(KPB1.GT.KM1-2.OR.KPB2.GT.KM2-2
     -   .OR.KPB3.GT.KM3-2)GOTO63
      DO349NV=2,NFB,2
      NVH=NV/2
      NFC=NFB-NV
      LPC=LCH(NFC+1)
      MDIC1=MIN0(3*NFC,3*(NMD-NFC))
      IF(IABS(KPB1-KPA1)+IABS(KPB2-KPA2)+
     -   IABS(KPB3-KPA3).GT.MDIC1)GOTO349
      MAXC1=KPA1+MDIC1
      MINC1=MAX0(KPA1-MDIC1,1)
      DO354KPC1=MINC1,KPB1
      MDIC2=MDIC1-IABS(KPC1-KPA1)
      MAXC2=KPA2+MDIC2
      MINC2=MAX0(KPA2-MDIC2,1)
  372 DO354KPC2=MINC2,MAXC2
      MDIC3=MDIC2-IABS(KPC2-KPA2)
      MAXC3=KPA3+MDIC3
      IN=1
      IS=KPAS+KPC1+KPC2+NFC
      IF(IS/2*2.EQ.IS)IN=2
      MINC3=MAX0(KPA3-MDIC3,IN)
      LO=KPC1.EQ.KPB1.AND.KPC2.EQ.KPB2.AND.NV.NE.NFB
      DO354KPC3=MINC3,MAXC3,2
      LPC=LPC+1
      IF(LO.AND.KPC3.EQ.KPB3)
     -   A=A+EN(NVH+2)*WFUN(LPC)
  354 CONTINUE
  349 CONTINUE
      IF(MVEX.LE.3)GOTO63
      NFBM=MIN0(NFB,MVEX-2)
      DO49NPART=1,3
      I=NPART+3
      AA1=AAA(I,1)
      AA2=AAA(I,2)
      AA3=AAA(I,3)
      AC1=AAA(I,4)
      AC2=AAA(I,5)
      AC3=AAA(I,6)
      DO70K1=1,KM1
      DO70K2=1,KM2
      DO70K3=1,KM3
   70 VX(K1,K2,K3)=0
      VX(KPB1+1,KPB2+1,KPB3+1)=1
      DO71IDEG=1,3
      MDB1=IDEG
      MIB1=MAX0(KPB1-MDB1,1)
      MAB1=MIN0(KPB1+MDB1,KM1-1)
      DO71KB1=MIB1,MAB1
      KB11=KB1+1
      KB12=KB1+2
      IF(KB12.GT.KM1)KB12=1
      AI1=AA1*(KB1+IK1)
      MDB2=MDB1-IABS(KB1-KPB1)
      MIB2=MAX0(KPB2-MDB2,1)
      MAB2=MIN0(KPB2+MDB2,KM2-1)
      DO71KB2=MIB2,MAB2
      KB21=KB2+1
      KB22=KB2+2
      IF(KB22.GT.KM2)KB22=1
      AI2=AA2*(KB2+IK2)
      IN=1
      IS=KPBS+KB1+KB2+IDEG
      IF(IS/2*2.EQ.IS)IN=2
      MDB3=MDB2-IABS(KB2-KPB2)
      MIB3=MAX0(KPB3-MDB3,IN)
      MAB3=MIN0(KPB3+MDB3,KM3-1)
      DO71KB3=MIB3,MAB3,2
      KB31=KB3+1
      KB32=KB3+2
      IF(KB32.GT.KM3)KB32=1
      AI3=AA3*(KB3+IK3)
      VX(KB11,KB21,KB31)=
     -   AI1*VX(KB12,KB21,KB31)+AC1*VX(KB1,KB21,KB31)+
     -   AI2*VX(KB11,KB22,KB31)+AC2*VX(KB11,KB2,KB31)+
     -   AI3*VX(KB11,KB21,KB32)+AC3*VX(KB11,KB21,KB3)
   31 FORMAT(A7,3I5,4D20.10)
   71 CONTINUE
      DO49NV=2,NFBM
      NVH=NV/2
      LO=NV.EQ.2*NVH
      NFC=NFB-NV
      LPC=LCH(NFC+1)
      MDIC1=MIN0(3*NFC,3*(NMD-NFC))
      MAXC1=KPA1+MDIC1
      MINC1=MAX0(KPA1-MDIC1,1)
      MDBC1=NV+2
      MAVC1=MIN0(MAXC1,KPB1+MDBC1)
      MIVC1=MAX0(MINC1,KPB1-MDBC1)
      IF(MIVC1.GT.MAVC1)GOTO49
      C=0
      DO54KPC1=MINC1,MAXC1
      MDBC2=MDBC1-IABS(KPC1-KPB1)
      MDIC2=MDIC1-IABS(KPC1-KPA1)
      MAXC2=KPA2+MDIC2
      MINC2=MAX0(KPA2-MDIC2,1)
      IF(MDBC2.LT.0)GOTO72
      KPC11=KPC1+1
      KPC12=KPC1+2
      AI1=AA1*(KPC1+IK1)
   72 DO54KPC2=MINC2,MAXC2
      MDBC3=MDBC2-IABS(KPC2-KPB2)
      MDIC3=MDIC2-IABS(KPC2-KPA2)
      MAXC3=KPA3+MDIC3
      IN=1
      IS=KPAS+KPC1+KPC2+NFC
      IF(IS/2*2.EQ.IS)IN=2
      MINC3=MAX0(KPA3-MDIC3,IN)
      IF(MDBC3.LT.0)GOTO73
      KPC21=KPC2+1
      KPC22=KPC2+2
      AI2=AA2*(KPC2+IK2)
   73 DO54KPC3=MINC3,MAXC3,2
      LPC=LPC+1
      MDBC=MDBC3-IABS(KPC3-KPB3)
      IF(MDBC.LT.0)GOTO54
      KPC31=KPC3+1
      KPC32=KPC3+2
      AI3=AA3*(KPC3+IK3)

               B=AI1*VX(KPC12,KPC21,KPC31)+AC1*VX(KPC1,
               KPC21,KPC31)
     -
               +AI2*VX(KPC11,KPC22,KPC31)+AC2*VX(KPC11,
               KPC2,KPC31)
     -
               +AI3*VX(KPC11,KPC21,KPC32)+AC3*VX(KPC11,
               KPC21,KPC3)
      VX(KPC11,KPC21,KPC31)=B
      C=C+B*WFUN(LPC)
   54 CONTINUE
      A=A-C*VEX(NPART,NV+3)
   49 CONTINUE
   63
               IF(KPB1.EQ.KPA1.AND.KPB2.EQ.KPA2.AND.KPB
               3.EQ.KPA3)
     -   GOTO64
      A=A/2/((KPB1-KPA1)*OM(1)+(KPB2-KPA2)*OM(2)
     -   +(KPB3-KPA3)*OM(3))
      GOTO62
   64 NFH=NFB/2
      EN(NFH+2)=-A
  500 FORMAT(A7,I5,(3D38.29))
  600 FORMAT(1x,A12,3i3,I5,(2D26.18))
      open(3,file='watch')
      write(3,600)'I123,
               ENERGY',ipa1,ipa2,ipa3,NFH,EN(NFH+2)
      close(3)
       IF(IPRI.GT.0)PRINT500,' ENERGY',NFH,EN(NFH+2)
      A=0
   62 WFUN(LPB)=A
   35 FORMAT(A7,5I5,4D20.10)
   51 CONTINUE
      LCH(NFB+2)=LPB
      IF(IPRI.GT.0)PRINT31,' LCH',NFB,LPB
  100 CONTINUE
      IF(IPRI.GT.0)PRINT92,' CF EN',(EN(I),I=1,NCOEF)
   92 FORMAT(A7,(3D40.29))
  994 FORMAT((1X,7('.',I4,I2,4I3)))
      RETURN
      END
      SUBROUTINE TAYLOR(X,VEX,NM,V,V1,V2,IFUN,PARAM)
      implicit complex*32(a-h,o-z)
      dimension
               X(3),VEX(3,99),V(99),V1(99),V2(99),PARAM
               (10)
      one=1
      DNU=PARAM(7)
      DO 1 I=1,3
      ZZ=PARAM(I)
      SCR=PARAM(I+3)
      DO 2 K=1,NM
      V2(K)=0
    2 V1(K)=0
      V1(1)=X(I)
      V1(2)=1
      CALL DEGPOL(V1,one/2,V,NM)
      GOTO(3,4,5,6),IFUN
    3 CALL DEGPOL(V,-one,V1,NM)
      CALL DEGPOL(V,DNU,V2,NM)
      GOTO99
    4 CALL DEGPOL(V,DNU,V1,NM)
      DO 11 K=1,NM
   11 V(K)=-SCR*V(K)
C      CALL EXPPOL(V,V2,NM)
      CALL PRPOL(V1,V2,V1,NM)
      DO 12 K=1,NM
   12 V2(K)=0
      GOTO99
    5 CALL PRPOL(V1,V1,V2,NM)
      GOTO99
    6 V(1)=V(1)+SCR
C      CALL LOGPOL(V,V1,NM)
      GOTO99
   99 DO 1 K=1,NM
    1 VEX(I,K)=V1(K)*ZZ+V2(K)*SCR
      RETURN
      END
      SUBROUTINE CONFRA(AA,A,B,C,N)
      IMPLICIT complex*32(A-H,O-Z)
      DIMENSION AA(N),A(N),B(N),C(N)
      DO1I=1,N
      IF(I.NE.1)GOTO2
      DO3K=1,N
      A(K)=AA(K)
    3 B(K)=0
      B(1)=1
      GOTO1
    2 KM=N-I+1
      A1=A(1)
      DO4K=1,KM
      B(K)=A(K)/A1
    4 A(K)=B(K+1)-A(K+1)/A1
    1 C(I)=A(1)
      RETURN
      END
      SUBROUTINE DEGPOL(A,P,B,N)
      IMPLICIT complex*32(A-H,O-Z)
      DIMENSION A(N),B(N)
      B(1)=A(1)**P
      IF(N.EQ.1)RETURN
      B(2)=P*A(2)*B(1)/A(1)
      IF(N.EQ.2)RETURN
      DO11I=3,N
      B(I)=P*(I-1)*A(I)*B(1)
      DO12K=3,I
      IK=I-K+2
   12 B(I)=B(I)+(K-2)*(P*A(K-1)*B(IK)-B(K-1)*A(IK))
   11 B(I)=B(I)/(I-1)/A(1)
      RETURN
      END
      complex*32 function padesum(a,x,n)
      implicit complex*32(a-h,o-z)
      dimension a(n),w1(100),w2(100),c(100)
      call confra(a,w1,w2,c,n)
      call volcfr(c,x,w1,w2,n)
      padesum=w1(n)/w2(n)
      return
      end
      SUBROUTINE PRPOL(A,B,C,N)
      IMPLICIT complex*32(A-H,O-Z)
      DIMENSION A(N),B(N),C(N)
      DO1I1=1,N
      I=N-I1+1
      D=0
      DO2K=1,I
      L=I-K+1
    2 D=D+A(K)*B(L)
    1 C(I)=D
      RETURN
      END
      SUBROUTINE VOLCFR(C,X,R,S,N)
      IMPLICIT complex*32(A-H,O-Z)
      DIMENSION C(N),R(N),S(N)
      DO1K=1,N
      IF(K.NE.1)GOTO2
      R(1)=C(1)
      S(1)=1
      GOTO1
    2 IF(K.NE.2)GOTO3
      R(2)=R(1)
      S(2)=S(1)+C(2)*X
      GOTO1
    3 R(K)=R(K-1)+C(K)*X*R(K-2)
      S(K)=S(K-1)+C(K)*X*S(K-2)
    1 CONTINUE
      RETURN
      END
      SUBROUTINE  MATIN2
               (A,DIM1,N1,DIM2,N2,INDEX,NERROR,DETERM)
               F1010000
C
               F1010010
C     MATRIX INVERSION WITH ACCOMPANYING SOLUTION OF
               LINEAR EQUATIONS.  F1010020
      complex*32      A,DETERM,DETER,PIVOT,SWAP
               F1010030
      INTEGER DIM1,DIM2,DIM,EMAT,PIVCOL,PIVC L1,PIVC L2
               F1010040
      DIMENSION A(DIM1),INDEX(DIM1)
               F1010050
c      DATA LGUNIT/51/
               F1010060
      DETER=1
               F1010070
      N=N1
               F1010080
      EMAT=N+N2
               F1010090
      DIM=DIM1
               F1010100
      NMIN1=N-1
               F1010110
C     THE ROUTINE DOES ITS OWN EVALUATION FOR DOUBLE
               SUBSCRIPTING OF    F1010120
C     ARRAY A.
               F1010130
      PIVCOL=1-DIM
               F1010140
C     MAIN LOOP TO INVERT THE MATRIX
               F1010150
      DO 11 MAIN=1,N
               F1010160
      PIVOT=0
               F1010170
      PIVCOL=PIVCOL+DIM
               F1010180
C     SEARCH FOR NEXT PIVOT IN COLUMN MAIN.
               F1010190
      PIVC L1=PIVCOL+MAIN-1
               F1010200
      PIVC L2=PIVCOL +NMIN1
               F1010210
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      DO 2 I1=PIVC L1,PIVC L2
                F1010220
      IF(ABS(A(I1))-ABS(PIVOT)) 2,2,1
                F1010230
    1 PIVOT=A(I1)
                F1010240
      LPIV=I1
                F1010250
    2 CONTINUE
                F1010260
C     IS PIVOT DIFFERENT FROM ZERO
                F1010270
      IF(ABS(PIVOT).LT.1.0E-12)GOTO 15
                F1010280
C     GET THE PIVOT-LINE INDICATOR AND SWAP LINES IF
                NECESSARY          F1010290
    3 ICOL=LPIV-PIVCOL+1
                F1010300
      INDEX(MAIN)=ICOL
                F1010310
      IF(ICOL-MAIN) 6,6,4
                F1010320
C     COMPLEMENT THE DETERMINANT
                F1010330
    4 DETER=-DETER
                F1010340
C     POINTER TO LINE PIVOT FOUND
                F1010350
      ICOL=ICOL-DIM
                F1010360
C     POINTER TO EXACT PIVOT LINE
                F1010370
      I3=MAIN-DIM
                F1010380
      DO 5 I=1,EMAT
                F1010390
      ICOL=ICOL+DIM
                F1010400
      I3=I3+DIM
                F1010410
      SWAP=A(I3)
                F1010420
      A(I3)=A(ICOL)
                F1010430
    5 A(ICOL)=SWAP
                F1010440
C     COMPUTE DETERMINANT
                F1010450
    6 DETER=DETER*PIVOT
                F1010460
      PIVOT=PIVOT**(-1)
                F1010470
C     TRANSFORM PIVOT COLUMN
                F1010480
      I3=PIVCOL+NMIN1
                F1010490
      DO 7 I=PIVCOL,I3
                F1010500
    7 A(I)=-A(I)*PIVOT
                F1010510
      A(PIVC L1)=PIVOT
                F1010520
C     PIVOT ELEMENT TRANSFORMED
                F1010530
C
                F1010540
C     NOW CONVERT REST OF THE MATRIX
                F1010550
      I1=MAIN-DIM
                F1010560
C     POINTER TO PIVOT LINE ELEMENTS
                F1010570
      ICOL=1-DIM
                F1010580
C     GENERAL COLUMN POINTER
                F1010590
      DO 10 I=1,EMAT
                F1010600
      ICOL=ICOL+DIM
                F1010610
      I1=I1+DIM
                F1010620
C     POINTERS MOVED
                F1010630
      IF(I-MAIN) 8,10,8
                F1010640
C     PIVOT COLUMN EXCLUDED
                F1010650
    8 JCOL=ICOL+NMIN1
                F1010660
      SWAP=A(I1)
                F1010670
      I3=PIVCOL-1
                F1010680
      DO 9 I2=ICOL,JCOL
                F1010690
      I3=I3+1
                F1010700
    9 A(I2)=A(I2)+SWAP*A(I3)
                F1010710
      A(I1)=SWAP*PIVOT
                F1010720
   10 CONTINUE
                F1010730
   11 CONTINUE
                F1010740
C     NOW REARRANGE THE MATRIX TO GET RIGHT INVERS
                F1010750
      DO 14 I1=1,N
                F1010760
      MAIN=N+1-I1
                F1010770
      LPIV=INDEX(MAIN)
                F1010780
      IF(LPIV-MAIN) 12,14,12
                F1010790
   12 ICOL=(LPIV-1)*DIM+1
                F1010800
      JCOL=ICOL+NMIN1
                F1010810
      PIVCOL=(MAIN-1)*DIM+1-ICOL
                F1010820
      DO 13 I2=ICOL,JCOL
                F1010830
      I3=I2+PIVCOL
                F1010840
      SWAP=A(I2)
                F1010850
      A(I2)=A(I3)
                F1010860
   13 A(I3)=SWAP
                F1010870
   14 CONTINUE
                F1010880
      DETERM=DETER
                F1010890
      NERROR=0
                F1010900
      RETURN
                F1010910
   15 NERROR=-1
                F1010920
      DETERM=DETER
                F1010930
c      WRITE(LGUNIT,100) MAIN,MAIN
                F1010940
      RETURN
                F1010950
  100 FORMAT(18H MATIN1 ..... THE ,I10,50H. COLUMN OF
                 THE MATRIX CONTAINF1010960
     1S ONLY ZEROS AT THE ,I10,19H. ELEMINATIONSSTEP. )
                F1010970
      END
                F1010980
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