technical memorandum Daresbury Laboratory

DL/SRF/TM 15
(Theory)

DIAGRAMMATIC MANY-BODY PERTURBATION EXPANSION FOR ATOMS AND MOLECULES: FORTRAN PROGRAM FOR CALCULATING FOURTH-ORDER, LINKED DIAGRAM ENERGY COMPONENTS INVOLVING QUADRUPLY-EXCITED STATES

by

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SEPTEMBER 1978

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1. INTRODUCTION

Programs for calculating electron correlation energies in small atoms and molecules, using the diagrammatic many-body perturbation expansion through third-order, have been described previously[1-5]. Beyond third-order, the fourth-order linked diagrams involving quadruply-excited intermediate states are of particular interest[5-9]. In a previous paper[6], we have described an algorithm for evaluating these energy components. The purpose of this note is to give the FORTRAN source code which was written to implement this algorithm, together with other programming details.

The programs are restricted to non-degenerate, closed-shell ground states of atoms and molecules. The reference wavefunction must be a matrix Hartree-Fock single determinantal function. The zero-order hamiltonian is taken to be the matrix Hartree-Fock operator.

In this note we refer to diagrams A-G of figure 1 in reference 6.

2. FORTRAN SOURCE CODE

The present program is code in FORTRAN IV. It consists of six routines:

MAIN in which the array I is dimensioned. This is of type INTEGER*4 and has a minimum dimension of 26 m^2, where m is the number of virtual orbitals.

QUAD is the controlling routine, in which the orbital energiss are processed, data set reference numbers are assigned, and printed output is produced.

UNPK is the routine which unpacks the labels assigned to the two electron integrals.

QU4A is the routine in which the energies corresponding to diagram A and the sum of diagrams F and G are evaluated.

QU4B controls the evaluation of the energies corresponding to the sum of diagrams B and C, and the sum of diagrams D and E.

RFST performs rapid read/write operations for arrays.

A complete listing of the FORTRAN source code is given in the Appendix. It should be noted the routines QU4A and QU4B may be overlaid.

3. INPUT DATA

There is no card input data for this program.

The following data files, which are generated by the third-order many-body perturbation expansion programs[1-4], are required:

19	(60)	title, orbital energies, etc.
20	(56)	primary file of "second-order" type integrals
21, 22, ...	(61, 62 ...)	secondary files of "second-order" type integrals

The figures in parentheses are the data set reference numbers assigned to these files in a previous Technical Memorandum[4].

4. STATUS

Illustrative applications of these programs may be found in the literature[6,9,10,11].

REFERENCES

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7. S. Wilson and D.M. Silver, Daresbury Laboratory Preprint DL/SRF/P146 (Theory) (1978) to appear to Comput. Phys. Commun.

8. S. Wilson and D.M. Silver, unpublished

9. S. Wilson and D.M. Silver, in Proc. Fourth Seminar on Computational Methods in Quantum Chemistry, Örenäs, Sweden, Sept. 1978, Daresbury Laboratory Preprint DL/SRF/P140 (Theory)

10. D.M. Silver, C.F. Bunge and S. Wilson, unpublished

11. S. Wilson and D.M. Silver, unpublished

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      DIMENSION I(130000)                                               00000010
      CALL QUAD(I)                                                      00000020
      STOP                                                              00000030
      END                                                               00000040
      SUBROUTINE QUAD(IW)                                               00000050
C***                                                                    00000060
C***                                                                    00000070
C***  PROGRAMS TO EVALUATE 4-TH ORDER ENERGY DIAGRAMS INVOLVING         00000080
C***  QUADRUPLY-EXCITED STATES.                                         00000090
C***  THESE PROGRAMS ARE RESTRICTED TO CLOSED-SHELL HARTREE-FOCK        00000100
C***  REFERENCE FUNCTIONS.                                              00000110
C***  CERTAIN DATA GENERATED BY THE MBPT PROGRAMS FOR THIRD-ORDER        00000120
C***  CALCULATIONS ARE REQUIRED AS INPUT.                               00000130
C***  IW(.) SHOULD BE OF TYPE INTEGER*4. IT SHOULD HAVE A DIMENSION     00000140
C***  OF AT LEAST 26*NVIRT**2, WHERE NVIRT IS THE NUMBER OF VIRTUAL     00000150
C***  ORBITALS.                                                         00000160
C***                                                                    00000170
C***                                                                    00000180
      IMPLICIT REAL*8 (A-H,O-Z)                                         00000190
      DIMENSION IW(1)                                                   00000200
      DIMENSION INVLAB(60)                                              00000210
      DIMENSION E(60),KTS(10),TITLE(10)                                 00000220
      DO 1 I=1,10                                                       00000230
      KTS(I)=20+I                                                       00000240
    1 CONTINUE                                                          00000250
      CALL ERRSET(208,256,-1,1,1,1)                                     00000260
C***                                                                    00000270
C***  INPUT...                                                          00000280
C***                                                                    00000290
      WRITE (6,1000)                                                    00000300
 1000 FORMAT(//1X,'FOURTH-ORDER ENERGY DIAGRAMS INVOLVING QUADR'        00000310
     &,'UPLY-EXCITED STATES')                                           00000320
      NT=19                                                             00000330
      READ(NT) TITLE,NOCC,NORB,E,INVLAB                                 00000340
      REWIND NT                                                         00000350
      NVIRT=NORB-NOCC                                                   00000360
      WRITE(6,1001) TITLE                                               00000370
 1001 FORMAT(/3X,10A8)                                                  00000380
      WRITE(6,1002) NOCC,NVIRT                                          00000390
 1002 FORMAT(/1X,'NUMBER OF OCCUPIED ORBITALS =',I3,                    00000400
     &       /1X,'NUMBER OF VIRTUAL  ORBITALS =',I3)                    00000410
      WRITE(6,1008)                                                     00000420
      DO 4 I=1,NORB                                                     00000429
      WRITE(6,1009) I,E(I)                                              00000430
    4 CONTINUE                                                          00000431
 1008 FORMAT(//1X,'ORBITAL ENERGIES'/)                                  00000440
 1009 FORMAT(5X,I2,3X,F13.7)                                            00000450
C***                                                                    00000460
C***  EVALUATE ENERGY CORRESPONDING TO DIAGRAMS A F G.                  00000470
C***                                                                    00000480
      DO 3 I=1,NOCC                                                     00000490
      KT=20+I                                                           00000500
      REWIND KT                                                         00000510
    3 CONTINUE                                                          00000520
      N=NVIRT*NVIRT                                                     00000530
      N2=N+N                                                            00000540
      N3=N2+N                                                           00000550
      N4=N3+N2                                                          00000560
      N5=N4+N                                                           00000570
      N6=N5+3*N2                                                        00000580
      N7=N6+3*N2                                                        00000590
      N8=N7+3*N2                                                        00000600
      N9=N8+N                                                           00000610
      CALL QU4A(E,NOCC,NVIRT,KTS,A,FG,IW(1),IW(N2+1),IW(N3+1),          00000620
     &IW(N4+1),IW(N5+1),IW(N6+1),IW(N7+1),IW(1),IW(N3+1),               00000630
     &IW(N8+1),IW(N9+1),N)                                              00000640
      DO 2 I=1,NOCC                                                     00000650
      KT=20+I                                                           00000660
      REWIND KT                                                         00000670
    2 CONTINUE                                                          00000680
C***                                                                    00000690
C***  EVALUATE ENERGY CORRESPONDING TO DIAGRAMS B C D E.                00000700
C***                                                                    00000710
      N6=N5+N2                                                          00000720
      N7=N6+N2                                                          00000730
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      N8=N7+N                                                           00000740
      NT=20                                                             00000750
      REWIND NT                                                         00000760
      READ(NT) TITLE                                                    00000770
      CALL QU4B(E,NOCC,NVIRT,NT,BC,DE,IW(1),IW(N2+1),IW(N3+1),          00000780
     &IW(N4+1),IW(N5+1),IW(N6+1),IW(1),IW(N3+1),IW(N7+1),               00000790
     &IW(N8+1),N)                                                       00000800
      REWIND NT                                                         00000810
C***                                                                    00000820
C***  OUTPUT                                                            00000830
C***                                                                    00000840
      BC=BC/8.0D+00                                                     00000850
      DE=-DE/2.0D+00                                                    00000860
      FG=-FG/2.0D+00                                                    00000870
      WRITE(6,1003) A                                                   00000880
      WRITE(6,1004) BC                                                  00000890
      WRITE(6,1005) DE                                                  00000900
      WRITE(6,1006) FG                                                  00000910
      WRITE(6,2341) A,BC,DE,FG                                          00000911
 2341 FORMAT(1X,4D26.16)                                                00000912
      T=A+BC+DE+FG                                                      00000920
      WRITE(6,1007) T                                                   00000930
 1003 FORMAT(//1X,'ENERGY CORRESPONDING TO DIAGRAM  A  ',F12.8)         00000940
 1004 FORMAT(   1X,'ENERGY CORRESPONDING TO DIAGRAMS B+C',F12.8)        00000950
 1005 FORMAT(   1X,'ENERGY CORRESPONDING TO DIAGRAMS D+E',F12.8)        00000960
 1006 FORMAT(   1X,'ENERGY CORRESPONDING TO DIAGRAMS F+G',F12.8)        00000970
 1007 FORMAT( /1X,'TOTAL ENERGY FOR DIAGRAMS             ',F12.8)      00000980
      RETURN                                                            00000990
      END                                                               00001000
      SUBROUTINE UNPK(IJ,N,L,NOCC,NVIRT)                                00001010
C***                                                                    00001020
C***   THIS PROGRAMME UNPACKS INTEGRAL LABELS.                          00001030
C***                                                                    00001040
      INTEGER IJ(N),L(NVIRT,NVIRT)                                      00001050
      DO 1 IA=1,NVIRT                                                   00001060
      DO 1 IB=1,NVIRT                                                   00001070
      L(IA,IB)=0                                                        00001080
    1 CONTINUE                                                          00001090
      DO 2 M=1,N                                                        00001100
      K=IJ(M)                                                           00001110
      IA=K/1200                                                         00001120
      IA=IA-(IA/60)*60-NOCC                                             00001130
      IB=K/20                                                           00001140
      IB=IB-(IB/60)*60-NOCC                                             00001150
      IT=K-(K/20)*20                                                    00001160
      GOTO (10,20,10,10,30),IT                                          00001170
   10 CONTINUE                                                          00001180
      L(IA,IB)=M                                                        00001190
      GOTO 60                                                           00001200
   20 CONTINUE                                                          00001210
      L(IA,IB)=M                                                        00001220
      L(IB,IA)=M                                                        00001230
      GOTO 60                                                           00001240
   30 CONTINUE                                                          00001250
      L(IB,IA)=M                                                        00001260
   60 CONTINUE                                                          00001270
    2 CONTINUE                                                          00001280
      RETURN                                                            00001290
      END                                                               00001300
      SUBROUTINE QU4A(E,NOCC,NVIRT,KTS,VA,VB,VIJ,MIJ,VJK,MJK,GA,        00001310
     &                GB,FA,NIJ,NJK,IJ,JK,NV)                           00001320
C***                                                                    00001330
C***  PROGRAMS TO EVALUATE 4-TH ORDER ENERGY DIAGRAMS INVOLVING         00001340
C***  QUADRUPLY-EXCITED STATES.                                         00001350
C***                                                                    00001360
C***  THIS SUBROUTINE EVALUATES DIAGRAMS A, F+G                         00001370
C***                                                                    00001380
C***     E(.)       ORBITAL ENERGIES                                    00001390
C***     NOCC       NUMBER OF OCCUPIED ORBITALS                         00001400
C***     NVIRT      NUMBER OF VIRTUAL ORBITALS                          00001410
C***     KTS(.)     DATA SET REFERENCE NUMBERS                          00001420
C***     VA         VALUE OF DIAGRAM A (RETURNED)                       00001430
C***     VB         VALUE OF DIAGRAMS F+G (RETURNED)                    00001440
C***                                                                    00001450
      IMPLICIT REAL*8 (A-H,O-Z)                                         00001460
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      LOGICAL*1 LIK,LIJ,LJK,LAJ,LAD                                     00001470
      DIMENSION VIJ(NV),VJK(NV),MIJ(NVIRT,NVIRT),MJK(NVIRT,NVIRT),      00001480
     & TA(3),TB(3),TD(3),                                               00001490
     & GA(NVIRT,NVIRT,3),GB(NVIRT,NVIRT,3),FA(NVIRT,NVIRT,3),           00001500
     & E(1),KTS(1)                                                      00001510
      DIMENSION NIJ(1),NJK(1)                                           00001520
      INTEGER IJ(NV),JK(NV)                                             00001530
      DATA Z/0.0D+00/                                                   00001540
C...                                                                    00001550
      WRITE(6,1000)                                                     00001560
 1000 FORMAT(//' BEGIN EVALUATION OF DIAGRAMS A, F+G')                  00001570
C...                                                                    00001580
      VA=Z                                                              00001590
      VB=Z                                                              00001600
C...                                                                    00001610
      DO 1 I=1,NOCC                                                     00001620
      IT=KTS(I)                                                         00001630
      DO 2 K=1,I                                                        00001640
      KT=KTS(K)                                                         00001650
      LIK=(I.EQ.K)                                                      00001660
C...                                                                    00001670
C...  TIK, TKI, SIK : INTERMEDIATES FOR DIAGRAMS F+G                   00001680
C...                                                                    00001690
      TIK=Z                                                             00001700
      TKI=Z                                                             00001710
      SIK=Z                                                             00001720
C...                                                                    00001730
C...  FA, GA, GB : INTERMEDIATES FOR DIAGRAM A                          00001740
C...                                                                    00001750
      DO 7 IB=1,NVIRT                                                   00001760
      DO 7 ID=1,NVIRT                                                   00001770
      DO 7 IS=1,3                                                       00001780
      FA(IB,ID,IS)=Z                                                    00001790
      GA(IB,ID,IS)=Z                                                    00001800
      GB(IB,ID,IS)=Z                                                    00001810
    7 CONTINUE                                                          00001820
C...                                                                    00001830
      DO 3 J=1,NOCC                                                     00001840
      LIJ=(I.EQ.J)                                                      00001850
      LJK=(J.EQ.K)                                                      00001860
      EIJ=E(I)+E(J)                                                     00001870
      EJK=E(J)+E(K)                                                     00001880
C...                                                                    00001890
C...  READ (IJ) BLOCK OF INTEGRALS                                     00001900
C...                                                                    00001910
      READ(IT) II,JJ,NN                                                 00001920
      NNN=NN+NN                                                         00001930
      CALL RFST(IJ,NN,IT)                                               00001940
      CALL RFST(NIJ,NNN,IT)                                             00001950
C...                                                                    00001960
C...  READ (JK) BLOCK OF INTEGRALS                                      00001970
C...                                                                    00001980
      IF(LIK) GOTO 12                                                   00001990
      READ(KT) JJ,KK,MM                                                 00002000
      IF(MM.EQ.0) GOTO 3                                                00002010
      MMM=MM+MM                                                         00002020
      CALL RFST(JK,MM,KT)                                               00002030
      CALL RFST(NJK,MMM,KT)                                             00002040
      GOTO 13                                                           00002050
   12 CONTINUE                                                          00002060
      MM=NN                                                             00002070
      DO 14 IZ=1,NN                                                     00002080
      VJK(IZ)=VIJ(IZ)                                                   00002090
      JK(IZ)=IJ(IZ)                                                     00002100
   14 CONTINUE                                                          00002110
   13 CONTINUE                                                          00002120
C...                                                                    00002130
C...  UNPACK LABELS...                                                  00002140
C...                                                                    00002150
      CALL UNPK(IJ,NN,MIJ,NOCC,NVIRT)                                   00002160
      CALL UNPK(JK,MM,MJK,NOCC,NVIRT)                                   00002170
C...                                                                    00002180
C...  SUM OVER J AND A FOR DIAGRAM A                                    00002190
C...                                                                    00002200
      DO 4 IB=1,NVIRT                                                   00002210
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      IIB=IB+NOCC                                                       00002220
      DO 5 ID=1,NVIRT                                                   00002230
      IID=ID+NOCC                                                       00002240
      DO 15 IZ=1,3                                                      00002250
      TA(IZ)=Z                                                          00002260
      TB(IZ)=Z                                                          00002270
      TD(IZ)=Z                                                          00002280
   15 CONTINUE                                                          00002290
      DO 6 IA=1,NVIRT                                                   00002300
      IIA=IA+NOCC                                                       00002310
      LAB=(IA.EQ.IB)                                                    00002320
      LAD=(IA.EQ.ID)                                                    00002330
      EAB=E(IIA)+E(IIB)                                                 00002340
      EAD=E(IIA)+E(IID)                                                 00002350
      DIJAB=EIJ-EAB                                                     00002360
      DJKAD=EJK-EAD                                                     00002370
      DJKAB=EJK-EAB                                                     00002380
      DIJAD=EIJ-EAD                                                     00002390
C                                                                       00002400
C     FIND <IJ/AB>, <IJ/BA>, <JK/DA>, <JK/AD>                           00002410
C                                                                       00002420
      I1=MIJ(IA,IB)                                                     00002430
      I2=MIJ(IB,IA)                                                     00002440
      J1=MIJ(IA,ID)                                                     00002450
      J2=MIJ(ID,IA)                                                     00002460
      K1=MJK(ID,IA)                                                     00002470
      K2=MJK(IA,ID)                                                     00002480
      L1=MJK(IB,IA)                                                     00002490
      L2=MJK(IA,IB)                                                     00002500
      IF(I1.EQ.0.AND.I2.EQ.0.AND.J1.EQ.0.AND.J2.EQ.0) GOTO 6            00002510
      IF(I1.EQ.0.AND.I2.EQ.0.AND.L1.EQ.0.AND.L2.EQ.0) GOTO 6            00002520
      IF(J1.EQ.0.AND.J2.EQ.0.AND.K1.EQ.0.AND.K2.EQ.0) GOTO 6            00002530
      IF(K1.EQ.0.AND.K2.EQ.0.AND.L1.EQ.0.AND.L2.EQ.0) GOTO 6            00002540
      IF(I.GE.J) GOTO 60                                                00002550
      ISAVE=I1                                                          00002560
      I1=I2                                                             00002570
      I2=ISAVE                                                          00002580
      ISAVE=J1                                                          00002590
      J1=J2                                                             00002600
      J2=ISAVE                                                          00002610
   60 CONTINUE                                                          00002620
      IF(J.GE.K) GOTO 61                                                00002630
      ISAVE=K1                                                          00002640
      K1=K2                                                             00002650
      K2=ISAVE                                                          00002660
      ISAVE=L1                                                          00002670
      L1=L2                                                             00002680
      L2=ISAVE                                                          00002690
   61 CONTINUE                                                          00002700
      P1=Z                                                              00002710
      P2=Z                                                              00002720
      Q1=Z                                                              00002730
      Q2=Z                                                              00002740
      R1=Z                                                              00002750
      R2=Z                                                              00002760
      S1=Z                                                              00002770
      S2=Z                                                              00002780
      IF(I1.NE.0) P1=VIJ(I1)                                            00002790
      IF(I2.NE.0) P2=VIJ(I2)                                            00002800
      IF(J1.NE.0) Q1=VIJ(J1)                                            00002810
      IF(J2.NE.0) Q2=VIJ(J2)                                            00002820
      IF(K1.NE.0) R1=VJK(K1)                                            00002830
      IF(K2.NE.0) R2=VJK(K2)                                            00002840
      IF(L1.NE.0) S1=VJK(L1)                                            00002850
      IF(L2.NE.0) S2=VJK(L2)                                            00002860
C                                                                       00002870
C                                                                       00002880
      IF(LIK) GOTO 23                                                   00002890
      IF(LJK.OR.LAB) GOTO 21                                            00002900
      IF(LIJ.OR.LAD) GOTO 20                                            00002910
      TD1=((S1-S2)*(Q1-Q2)+S2*Q2)/DJKAB                                 00002920
      TD2=((S1-S2)*Q2+S2*(Q1-Q2))/DJKAB                                 00002930
      TD3=S1*Q1/DJKAB                                                   00002940
      GOTO 24                                                           00002950
   20 CONTINUE                                                          00002960
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      TD1=S2*Q2/DJKAB                                                   00002970
      TD2=(S1-S2)*Q2/DJKAB                                              00002980
      TD3=S1*Q1/DJKAB                                                   00002990
      GOTO 24                                                           00003000
   21 CONTINUE                                                          00003010
      IF(LIJ.OR.LAD) GOTO 22                                            00003020
      TD1=S2*Q2/DJKAB                                                   00003030
      TD2=S2*(Q1-Q2)/DJKAB                                              00003040
      TD3=S1*Q1/DJKAB                                                   00003050
      GOTO 24                                                           00003060
   22 CONTINUE                                                          00003070
      TD1=S2*Q2/DJKAB                                                   00003080
      TD2=Z                                                             00003090
      TD3=S1*Q1/DJKAB                                                   00003100
   24 CONTINUE                                                          00003110
   23 CONTINUE                                                          00003120
      IF(LJK.OR.LAD) GOTO 25                                            00003130
      IF(LIJ.OR.LAB) GOTO 26                                            00003140
      TB1=((P1-P2)*(R1-R2)+P2*R2)/DIJAB                                 00003150
      TB2=((P1-P2)*R2+P2*(R1-R2))/DIJAB                                 00003160
      TB3=P1*R1/DIJAB                                                   00003170
      GOTO 27                                                           00003180
   26 CONTINUE                                                          00003190
      TB1=P2*R2/DIJAB                                                   00003200
      TB2=P2*(R1-R2)/DIJAB                                              00003210
      TB3=P1*R1/DIJAB                                                   00003220
      GOTO 27                                                           00003230
   25 CONTINUE                                                          00003240
      IF(LIJ.OR.LAB) GOTO 28                                            00003250
      TB1=P2*R2/DIJAB                                                   00003260
      TB2=(P1-P2)*R2/DIJAB                                              00003270
      TB3=P1*R1/DIJAB                                                   00003280
      GOTO 27                                                           00003290
   28 CONTINUE                                                          00003300
      TB1=P2*R2/DIJAB                                                   00003310
      TB2=Z                                                             00003320
      TB3=P1*R1/DIJAB                                                   00003330
   27 CONTINUE                                                          00003340
C...                                                                    00003350
      TA1=TB1/DJKAD                                                     00003360
      TA2=TB2/DJKAD                                                     00003370
      TA3=TB3/DJKAD                                                     00003380
      TA(1)=TA(1)+TA1                                                   00003390
      TA(2)=TA(2)+TA2                                                   00003400
      TA(3)=TA(3)+TA3                                                   00003410
      TB(1)=TB(1)+TB1                                                   00003420
      TB(2)=TB(2)+TB2                                                   00003430
      TB(3)=TB(3)+TB3                                                   00003440
      IF(LIK) GOTO 6                                                    00003450
      TD(1)=TD(1)+TD1                                                   00003460
      TD(2)=TD(2)+TD2                                                   00003470
      TD(3)=TD(3)+TD3                                                   00003480
    6 CONTINUE                                                          00003490
      DO 8 IS=1,3                                                       00003500
      FA(IB,ID,IS)=TA(IS)+FA(IB,ID,IS)                                  00003510
      GA(IB,ID,IS)=TB(IS)+GA(IB,ID,IS)                                  00003520
      IF(LIK) GOTO 8                                                    00003530
      GB(IB,ID,IS)=TD(IS)+GB(IB,ID,IS)                                  00003540
    8 CONTINUE                                                          00003550
    5 CONTINUE                                                          00003560
    4 CONTINUE                                                          00003570
C...                                                                    00003580
C...  SUM OVER A AND B FOR DIAGRAMS F+G                                 00003590
C...                                                                    00003600
      DO 50 IA=1,NVIRT                                                  00003610
      IIA=IA+NOCC                                                       00003620
      DO 51 IB=1,NVIRT                                                  00003630
      LAB=(IA.EQ.IB)                                                    00003640
      IIB=IB+NOCC                                                       00003650
      EAB=E(IIA)+E(IIB)                                                 00003660
      DIJAB=EIJ-EAB                                                     00003670
      DJKAB=EJK-EAB                                                     00003680
C...                                                                    00003690
C...  FIND <IJ/AB>, <IJ/BA>, <JK/AB>, <JK/BA>                          00003700
C...                                                                    00003710
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      I1=MIJ(IA,IB)                                                     00003720
      I2=MIJ(IB,IA)                                                     00003730
      J1=MJK(IB,IA)                                                     00003740
      J2=MJK(IA,IB)                                                     00003750
      IF(I1.EQ.0.AND.I2.EQ.0) GOTO 51                                   00003760
      IF(J1.EQ.0.AND.J2.EQ.0) GOTO 51                                   00003770
      IF(I.GE.J) GOTO 52                                                00003780
      ISAVE=I1                                                          00003790
      I1=I2                                                             00003800
      I2=ISAVE                                                          00003810
   52 CONTINUE                                                          00003820
      IF(J.GE.K) GOTO 53                                                00003830
      ISAVE=J1                                                          00003840
      J1=J2                                                             00003850
      J2=ISAVE                                                          00003860
   53 CONTINUE                                                          00003870
      P1=Z                                                              00003880
      P2=Z                                                              00003890
      Q1=Z                                                              00003900
      Q2=Z                                                              00003910
      IF(I1.NE.0) P1=VIJ(I1)                                            00003920
      IF(I2.NE.0) P2=VIJ(I2)                                            00003930
      IF(J1.NE.0) Q1=VJK(J1)                                            00003940
      IF(J2.NE.0) Q2=VJK(J2)                                            00003950
C                                                                       00003960
      IF(LIJ.OR.LJK.OR.LAB) GOTO 30                                     00003970
      T=(P1-P2)*(Q1-Q2)+P1*Q1+P2*Q2                                     00003980
      TIK=TIK+T/DIJAB                                                   00003990
      IF(LIK) GOTO 31                                                   00004000
      TKI=TKI+T/DJKAB                                                   00004010
   31 CONTINUE                                                          00004020
      SIK=SIK+T/(DJKAB*DIJAB)                                           00004030
      GOTO 32                                                           00004040
   30 CONTINUE                                                          00004050
      T=P1*Q1+P2*Q2                                                     00004060
      TIK=TIK+T/DIJAB                                                   00004070
      IF(LIK) GOTO 33                                                   00004080
      TKI=TKI+T/DJKAB                                                   00004090
   33 CONTINUE                                                          00004100
      SIK=SIK+T/(DJKAB*DIJAB)                                           00004110
   32 CONTINUE                                                          00004120
   51 CONTINUE                                                          00004130
   50 CONTINUE                                                          00004140
C                                                                       00004150
    3 CONTINUE                                                          00004160
      REWIND IT                                                         00004170
      REWIND KT                                                         00004180
C                                                                       00004190
C     COMPLETE EVALUATION OF DIAGRAM A                                  00004200
C                                                                       00004210
      DO 9 IB=1,NVIRT                                                   00004220
      DO 10 ID=1,NVIRT                                                  00004230
      DO 11 IS=1,3                                                      00004240
      VA=FA(IB,ID,IS)*GA(IB,ID,IS)+VA                                   00004250
      IF(LIK) GOTO 11                                                   00004260
      VA=FA(ID,IB,IS)*GB(IB,ID,IS)+VA                                   00004270
   11 CONTINUE                                                          00004280
   10 CONTINUE                                                          00004290
    9 CONTINUE                                                          00004300
C                                                                       00004310
C     COMPLETE EVALUATION OF DIAGRAMS F+G                               00004320
C                                                                       00004330
      VB=SIK*(TIK+TKI)+VB                                               00004340
    2 CONTINUE                                                          00004350
    1 CONTINUE                                                          00004360
C                                                                       00004370
      WRITE(6,1001)                                                     00004380
 1001 FORMAT(//' EVALUATION OF DIAGRAMS A, F+G COMPLETED')              00004390
C                                                                       00004400
      RETURN                                                            00004410
      END                                                               00004420
      SUBROUTINE QU4B(E,NOCC,NVIRT,NT,VA,VB,VIJ,MIJ,VKL,MKL,            00004430
     &                GDE,FDE,NIJ,NKL,IJ,KL,NV)                         00004440
C                                                                       00004450
C     PROGRAMS TO EVALUATE 4-TH ORDER ENERGY DIAGRAMS INVOLVING         00004460
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C...   QUADRUPLY-EXCITED STATES.                                                00004470
C...                                                                           00004480
C...   THIS SUBROUTINE EVALUATES DIAGRAMS B+C, D+E                             00004490
C...                                                                           00004500
C...      E(.)        ORBITAL ENERGIES                                         00004510
C...      NOCC        NUMBER OF OCCUPIED ORBITALS                              00004520
C...      NVIRT       NUMBER OF VIRTUAL ORBITALS                               00004530
C...      NT          DATA SET REFERENCE NUMBER                                00004540
C...      VA          VALUES OF DIAGRAMS B+C (RETURNED)                        00004550
C...      VB          VALUES OF DIAGRAMS D+E (RETURNED)                        00004560
C...                                                                           00004570
      IMPLICIT REAL*8 (A-H,O-Z)                                                00004580
      DIMENSION E(1),FBC(3),GBC(3),FDE(NVIRT,NVIRT),GDE(NVIRT,NVIRT),          00004590
     &MIJ(NVIRT,NVIRT),MKL(NVIRT,NVIRT)                                        00004600
      DIMENSION VIJ(NV),VKL(NV)                                                00004610
      LOGICAL*1 LIJ,LJL,LIK,LKL,LAC,LAB,LBC                                    00004620
      DIMENSION NIJ(1),NKL(1)                                                  00004630
      INTEGER IJ(NV),KL(NV)                                                    00004640
      DIMENSION DUMMY(10)                                                      00004650
      DATA Z/0.0D+00/                                                          00004660
C...                                                                           00004670
      WRITE(6,1000)                                                            00004680
 1000 FORMAT(//' BEGIN EVALUATION OF DIAGRAMS B+C, D+E')                       00004690
C...                                                                           00004700
      VA=Z                                                                     00004710
      VB=Z                                                                     00004720
C...                                                                           00004730
C...   FDE, GDE :- INTERMEDIATES FOR DIAGRAMS D+E                              00004740
C...                                                                           00004750
      DO 5 IA=1,NVIRT                                                          00004760
      DO 5 IC=1,NVIRT                                                          00004770
      FDE(IA,IC)=Z                                                             00004780
      GDE(IA,IC)=Z                                                             00004790
    5 CONTINUE                                                                 00004800
C...                                                                           00004810
      DO 1 I=1,NOCC                                                            00004820
      DO 1 J=1,I                                                               00004830
      LIJ=(I.EQ.J)                                                             00004840
C...                                                                           00004850
C...   READ (IJ) BLOCK OF INTEGRALS                                            00004860
C...                                                                           00004870
      READ(NT) II,JJ,NN                                                        00004880
      NNN=NN+NN                                                                00004890
      CALL RFST(IJ,NN,NT)                                                      00004900
      CALL RFST(NIJ,NNN,NT)                                                    00004910
      REWIND NT                                                                00004920
      READ(NT) DUMMY                                                           00004930
      CALL UNPK(IJ,NN,MIJ,NOCC,NVIRT)                                          00004940
      EIJ=E(I)+E(J)                                                            00004950
C...                                                                           00004960
      DO 2 K=1,I                                                               00004970
      LIK=(I.EQ.K)                                                             00004980
      DO 2 L=1,K                                                               00004990
      LJL=(J.EQ.L)                                                             00005000
      LKL=(K.EQ.L)                                                             00005010
      IF(LIK.AND.L.GT.J) GOTO 2                                                00005020
C...                                                                           00005030
C...   READ (KL) BLOCK OF INTEGRALS                                            00005040
C...                                                                           00005050
      READ(NT) KK,LL,MM                                                        00005060
      MMM=MM+MM                                                                00005070
      CALL RFST(KL,MM,NT)                                                      00005080
      CALL RFST(NKL,MMM,NT)                                                    00005090
      CALL UNPK(KL,MM,MKL,NOCC,NVIRT)                                          00005100
      EKL=E(K)+E(L)                                                            00005110
C...                                                                           00005120
C...   SUM OVER A AND B FOR DIAGRAMS B+C                                       00005130
C...                                                                           00005140
      F1=Z                                                                     00005150
      F2=Z                                                                     00005160
      F3=Z                                                                     00005170
      GA1=Z                                                                    00005180
      GA2=Z                                                                    00005190
      GA3=Z                                                                    00005200
      GB1=Z                                                                    00005210
```

```
      GB2=Z                                                             00005220
      GB3=Z                                                             00005230
      DO 3 IA=1,NVIRT                                                   00005240
      IIA=IA+NOCC                                                       00005250
      DO 3 IB=1,NVIRT                                                   00005260
      IIB=IB+NOCC                                                       00005270
      LAB=(IA.EQ.IB)                                                    00005280
      EAB=E(IIA)+E(IIB)                                                 00005290
      DIJAB=EIJ-EAB                                                     00005300
      DKLAB=EKL-EAB                                                     00005310
C                                                                       00005320
C     FIND <IJ/AB>, <IJ/BA>, <KL/AB>, <KL/BA>                           00005330
C                                                                       00005340
      I1=MIJ(IA,IB)                                                     00005350
      I2=MIJ(IB,IA)                                                     00005360
      J1=MKL(IA,IB)                                                     00005370
      J2=MKL(IB,IA)                                                     00005380
      IF(I1.EQ.0.AND.I2.EQ.0) GOTO 3                                    00005390
      IF(J1.EQ.0.AND.J2.EQ.0) GOTO 3                                    00005400
      P1=Z                                                              00005410
      P2=Z                                                              00005420
      Q1=Z                                                              00005430
      Q2=Z                                                              00005440
      IF(I1.NE.0) P1=VIJ(I1)                                            00005450
      IF(I2.NE.0) P2=VIJ(I2)                                            00005460
      IF(J1.NE.0) Q1=VKL(J1)                                            00005470
      IF(J2.NE.0) Q2=VKL(J2)                                            00005480
C                                                                       00005490
      T1=Z                                                              00005500
      IF(LAB.OR.LIJ.OR.LKL) GOTO 41                                     00005510
      T1=(P1-P2)*(Q1-Q2)                                                00005520
   41 T2=P1*Q1+P2*Q2                                                    00005530
      T3=P1*Q2+P2*Q1                                                    00005540
      GA1=GA1+T1/DIJAB                                                  00005550
      GA2=GA2+T2/DIJAB                                                  00005560
      GA3=GA3+T3/DIJAB                                                  00005570
      GB1=GB1+T1/DKLAB                                                  00005580
      GB2=GB2+T2/DKLAB                                                  00005590
      GB3=GB3+T3/DKLAB                                                  00005600
      D=DIJAB*DKLAB                                                     00005610
      F1=F1+T1/D                                                        00005620
      F2=F2+T2/D                                                        00005630
      F3=F3+T3/D                                                        00005640
    3 CONTINUE                                                          00005650
C                                                                       00005660
C     COMPLETE EVALUATION OF DIAGRAMS B+C                               00005670
C                                                                       00005680
      KKL=1                                                             00005690
      KIJ=1                                                             00005700
      IF(LKL) KKL=0                                                     00005710
      IF(LIJ) KIJ=0                                                     00005720
      N1=(1+KIJ)*(1+KKL)                                                00005730
      N2=N1                                                             00005740
      IF(LIK.AND.LJL) N2=0                                              00005750
      VA=DFLOAT(N1)*(GA1*F1+GA2*F2+GA3*F3)+                             00005760
     &   DFLOAT(N2)*(GB1*F1+GB2*F2+GB3*F3)                              00005770
     &   + VA                                                           00005780
    2 CONTINUE                                                          00005790
C                                                                       00005800
C     SUM OVER I,J,B FOR DIAGRAMS D+E                                   00005810
C                                                                       00005820
      DO 6 IA=1,NVIRT                                                   00005830
      IIA=IA+NOCC                                                       00005840
      DO 6 IC=1,IA                                                      00005850
      IIC=IC+NOCC                                                       00005860
      LAC=(IA.EQ.IC)                                                    00005870
      DO 7 IB=1,NVIRT                                                   00005880
      IIB=IB+NOCC                                                       00005890
      EAB=E(IIA)+E(IIB)                                                 00005900
      EBC=E(IIB)+E(IIC)                                                 00005910
      DIJAB=EIJ-EAB                                                     00005920
      DIJBC=EIJ-EBC                                                     00005930
      LAB=(IA.EQ.IB)                                                    00005940
      LBC=(IB.EQ.IC)                                                    00005950
C                                                                       00005960
```

```
C...  FIND <IJ/AB>, <IJ/BA>, <IJ/CB>, <IJ/BC>                          00005970
C...                                                                  00005980
      I1=MIJ(IA,IB)                                                   00005990
      I2=MIJ(IB,IA)                                                   00006000
      J1=MIJ(IC,IB)                                                   00006010
      J2=MIJ(IB,IC)                                                   00006020
      IF(I1.EQ.0.AND.I2.EQ.0) GOTO 7                                  00006030
      IF(J1.EQ.0.AND.J2.EQ.0) GOTO 7                                  00006040
      P1=Z                                                            00006050
      P2=Z                                                            00006060
      Q1=Z                                                            00006070
      Q2=Z                                                            00006080
      IF(I1.NE.0) P1=VIJ(I1)                                          00006090
      IF(I2.NE.0) P2=VIJ(I2)                                          00006100
      IF(J1.NE.0) Q1=VIJ(J1)                                          00006110
      IF(J2.NE.0) Q2=VIJ(J2)                                          00006120
C...                                                                  00006130
      IF(LIJ.OR.LAB.OR.LBC) GOTO 60                                   00006140
      T=(P1-P2)*(Q1-Q2)+P1*Q1+P2*Q2                                   00006150
      T=T+T                                                           00006160
      GDE(IA,IC)=GDE(IA,IC)+T/DIJAB                                   00006170
      IF(.NOT.LAC) GDE(IC,IA)=GDE(IC,IA)+T/DIJBC                      00006180
      FDE(IA,IC)=FDE(IA,IC)+T/(DIJAB*DIJBC)                           00006190
      GOTO 61                                                         00006200
   60 CONTINUE                                                        00006210
      T=P1*Q1+P2*Q2                                                   00006220
      IF(.NOT.LIJ) T=T+T                                              00006230
      GDE(IA,IC)=GDE(IA,IC)+T/DIJAB                                   00006240
      IF(.NOT.LAC) GDE(IC,IA)=GDE(IC,IA)+T/DIJBC                      00006250
      FDE(IA,IC)=FDE(IA,IC)+T/(DIJAB*DIJBC)                           00006260
   61 CONTINUE                                                        00006270
    7 CONTINUE                                                        00006280
    6 CONTINUE                                                        00006290
C...                                                                  00006300
    1 CONTINUE                                                        00006310
C...                                                                  00006320
C...  COMPLETE EVALUATION OF DIAGRAMS D+E                             00006330
C...                                                                  00006340
      DO 9 IC=2,NVIRT                                                 00006350
      IIA=IC-1                                                        00006360
      DO 9 IA=1,IIA                                                   00006370
      FDE(IA,IC)=FDE(IC,IA)                                           00006380
    9 CONTINUE                                                        00006390
      DO 8 IA=1,NVIRT                                                 00006400
      DO 8 IC=1,NVIRT                                                 00006410
      VB=FDE(IA,IC)*GDE(IA,IC)+VB                                     00006420
    8 CONTINUE                                                        00006430
C...                                                                  00006440
C...                                                                  00006450
      WRITE(6,1001)                                                   00006460
 1001 FORMAT(//' EVALUATION OF DIAGRAMS B+C, D+E COMPLETED')          00006470
      RETURN                                                          00006480
      END                                                             00006490
      SUBROUTINE WEST(I,N,KT)                                         00006500
C...  THIS PROGRAMME PERFORMS RAPID READ/WRITE OPERATIONS.            00006510
      INTEGER I(N)                                                    00006520
      READ(KT) I                                                      00006530
      RETURN                                                          00006540
      ENTRY WEST(I,N,KT)                                              00006550
      WRITE(KT) I                                                     00006560
      RETURN                                                          00006570
      END                                                             00006580
```