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DIAGRAMMATIC MANY-BODY PERTURBATION EXPANSION FOR ATOMS AND MOLECULES:

FORTRAN PROGRAM FOR CALCULATING FOURTH-ORDER, LINKED DIAGRAM

ENERGY COMPONENTS INVOLVING QUADRUPLY-EXCITED STATES

by

S. WILSON, Daresbury Laboratory

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Science Research Council

Daresbury Laboratory

Daresbury, Warrington WA4 4AD

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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).

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DIMENSION I(130000) 00000010
CALL QUAD(I) 00000020
STOP 00000030
END 00000040
SUBROUTINE QUAD(IW) 00000050
...
*** PROGRAMS TO EVALUATE 4-TH ORDER ENERGY DIAGRAMS INVOLVING 00000060
*** QUADRUPLY-EXCITED STATES. 00000070
*** THESE PROGRAMS ARE RESTRICTED TO CLOSED-SHELL HARTREE-FOCK 00000080
*** REFERENCE FUNCTIONS. 00000090
*** CERTAIN DATA GENERATED BY THE MBPT PROGRAMS FOR THIRD-ORDER 00000100
*** CALCULATIONS ARE REQUIRED AS INPUT. 00000110
*** IW(.) SHOULD BE OF TYPE INTEGER*4. IT SHOULD HAVE A DIMENSION 00000120
*** OF AT LEAST 26*NVIRT**2, WHERE NVIRT IS THE NUMBER OF VIRTUAL 00000130
*** ORBITALS. 00000140
...
*** IMPLICIT REAL*8 (A-H,O-Z) 00000150
DIMENSION IW(1) 00000160
DIMENSION INVLAB(60) 00000170
DIMENSION E(60),KTS(10),TITLE(10) 00000180
DO 1 I=1,10 00000190
KTS(I)=20+I 00000200
1 CONTINUE 00000210
CALL ERRSET(208,256,-1,1,1,1) 00000220
...
*** INPUT...
...
1000 WRITE (6,1000) 00000230
FORMAT(//1X,'FOURTH-ORDER ENERGY DIAGRAMS INVOLVING QUADR*' 00000240
&,'UPLY-EXCITED STATES') 00000250
NT=19 00000260
READ(NT) TITLE,NOCC,NORB,E,INVLAB 00000270
REWIND NT 00000280
NVIRT=NORB-NOCC 00000290
1001 WRITE(6,1001) TITLE 00000300
FORMAT(/3X,10A8) 00000310
1002 WRITE(6,1002) NOCC,NVIRT 00000320
& FORMAT(/1X,'NUMBER OF OCCUPIED ORBITALS =',I3, 00000330
/1X,'NUMBER OF VIRTUAL ORBITALS =',I3) 00000340
WRITE(6,1008) 00000350
DO 4 I=1,NJRB 00000360
WRITE(6,1009) I,E(I) 00000370
4 CONTINUE 00000380
1008 FORMAT(//1X,'ORBITAL ENERGIES') 00000390
1009 FORMAT(5X,I2,3X,F13.7) 00000400
...
*** EVALUATE ENERGY CORRESPONDING TO DIAGRAMS A F G. 00000410
...
DO 3 I=1,NOCC 00000420
KT=20+I 00000430
REWIND KT 00000440
3 CONTINUE 00000450
N=NVIRT*NVIRT 00000460
N2=N+N 00000470
N3=N2+N 00000480
N4=N3+N2 00000490
N5=N4+N 00000500
N6=N5+3*N2 00000510
N7=N6+3*N2 00000520
N8=N7+3*N2 00000530
N9=N8+N 00000540
CALL QU4A(E,NOCC,NVIRT,KTS,A,FG,IW(1),IW(N2+1),IW(N3+1), 00000550
&IW(N4+1),IW(N5+1),IW(N6+1),IW(N7+1),IW(1),IW(N3+1), 00000560
&IW(N8+1),IW(N9+1),N) 00000570
DO 2 I=1,NOCC 00000580
KT=20+I 00000590
REWIND KT 00000600
2 CONTINUE 00000610
...
*** EVALUATE ENERGY CORRESPONDING TO DIAGRAMS B C D E. 00000620
...
N6=N5+N2 00000630
N7=N6+N2 00000640
N8=N7+N2 00000650
N9=N8+N 00000660

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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),
&IW(N4+1),IW(N5+1),IW(N6+1),IW(1),IW(N3+1),IW(N7+1),
&IW(N8+1),N)   00000780
REWIND NT        00000810
*** OUTPUT       00000820
***               00000830
BC=BC/8.0D+00    00000840
DE=-DE/2.0D+00   00000850
FG=-FG/2.0D+00   00000860
WRITE(6,1003) A  00000870
WRITE(6,1004) BC 00000880
WRITE(6,1005) DE 00000890
WRITE(6,1006) FG 00000910
2341 WRITE(6,2341) A,BC,DE,FG 00000911
FORMAT(IX,4D26.16) 00000912
T=A+3C+DE+FG   00000920
WRITE(6,1007) T  00000930
1003 FORMAT(//IX,'ENERGY CORRESPONDING TO DIAGRAM A ',F12.8) 00000940
1004 FORMAT(//IX,'ENERGY CORRESPONDING TO DIAGRAMS B+C ',F12.8) 00000950
1005 FORMAT(//IX,'ENERGY CORRESPONDING TO DIAGRAMS D+E ',F12.8) 00000960
1006 FORMAT(//IX,'ENERGY CORRESPONDING TO DIAGRAMS F+G ',F12.8) 00000970
1007 FORMAT(//IX,'TOTAL ENERGY FOR DIAGRAMS ',F12.8) 00000980
RETURN          00000990
END             00001000
SUBROUTINE UNPK(IJ,N,L,NOCC,NVIRT) 00001010
*** THIS PROGRAMME UNPACKS INTEGRAL LABELS. 00001020
***               00001030
INTEGER IJ(N),L(NVIRT,NVIRT) 00001040
DO 1 IA=1,NVIRT 00001050
DO 1 IB=1,NVIRT 00001060
L(IA,IB)=0 00001070
1 CONTINUE        00001080
DO 2 M=1,N 00001090
K=IJ(M) 00001100
IA=K/1200 00001110
IA=IA-(IA/60)*60-NOCC 00001120
IB=K/20 00001130
IB=IB-(IB/60)*60-NOCC 00001140
IT=K-(K/20)*20 00001150
GOTO (10,20,10,10,30),IT 00001160
10 CONTINUE        00001170
L(IA,IB)=M 00001180
GOTO 60 00001190
20 CONTINUE        00001200
L(IA,IB)=M 00001210
L(IB,IA)=M 00001220
GOTO 60 00001230
30 CONTINUE        00001240
L(IB,IA)=M 00001250
60 CONTINUE        00001260
2 CONTINUE         00001270
RETURN          00001280
END             00001290
SUBROUTINE QU4A(E,NOCC,NVIRT,KTS,VA,VB,VIJ,MIJ,VJK,MJK,GA,
& GB,FA,NIJ,NJK,IJ,JK,NV) 00001300
&               00001310
*** PROGRAMS TO EVALUATE 4-TH ORDER ENERGY DIAGRAMS INVOLVING 00001320
*** QUADRUPLY-EXCITED STATES. 00001330
***               00001340
*** THIS SUBROUTINE EVALUATES DIAGRAMS A, F+G 00001350
***               00001360
E(.) ORBITAL ENERGIES 00001370
NOCC NUMBER OF OCCUPIED ORBITALS 00001380
NVIRT NUMBER OF VIRTUAL ORBITALS 00001390
KTS(.) DATA SET REFERENCE NUMBERS 00001400
VA VALUE OF DIAGRAM A (RETURNED) 00001410
VB VALUE OF DIAGRAMS F+G (RETURNED) 00001420
IMPLICIT REAL*8 (A-H,O-Z) 00001430
00001440
00001450
00001460

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LOGICAL*1 LIK,LIJ,LJK,LA3,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...
      WRITE(6,1000)                      00001550
1000 FORMAT(//' BEGIN EVALUATION OF DIAGRAMS A, F+G')
C...
      VA=Z                            00001560
      VB=Z                            00001570
C...
      DO 1 I=1,NOCC                   00001580
      IT=KTS(I)
      DO 2 K=1,I                     00001590
      KT=KTS(K)
      LIK=(I.EQ.K)                  00001600
C...
      TIK, TKI, SIK : INTERMEDIATES FOR DIAGRAMS F+G 00001610
C...
      TIK=Z                           00001620
      TKI=Z                           00001630
      SIK=Z                           00001640
C...
      LIK=Z                           00001650
C...
      FA, GA, GB : INTERMEDIATES FOR DIAGRAM A   00001660
C...
      DO 7 IB=1,NVIRT                 00001670
      DO 7 ID=1,NVIRT                 00001680
      DO 7 IS=1,3                    00001690
      FA(IB,ID,IS)=Z               00001700
      GA(IB,ID,IS)=Z               00001710
      GB(IB,ID,IS)=Z               00001720
      7 CONTINUE                      00001730
C...
      DO 3 J=1,NOCC                   00001740
      LIJ=(I.EQ.J)
      LJK=(J.EQ.K)
      EIJ=E(I)+E(J)
      EJK=E(J)+E(K)
C...
      READ (IJ) BLOCK OF INTEGRALS 00001750
C...
      READ(IT) II,JJ,NN              00001760
      NNN=NN+NN                      00001770
      CALL RFST(IJ,NN,IT)            00001780
      CALL RFST(NIJ,NNN,IT)          00001790
C...
      READ (JK) BLOCK OF INTEGRALS 00001800
C...
      IF(LIK) GOTO 12                00001810
      READ(KT) JJ,MM,MM              00001820
      IF(MM.EQ.0) GOTO 3             00001830
      MMM=MM+MM                      00001840
      CALL RFST(JK,MM,KT)            00001850
      CALL RFST(NJK,MMM,KT)          00001860
      GOTO 13                         00001870
12 CONTINUE                      00001880
      MM=NN                          00001890
      DO 14 IZ=1,NN                  00001900
      VJK(IZ)=VIJ(IZ)                00001910
      JK(IZ)=IJ(IZ)                  00001920
14 CONTINUE                      00001930
13 CONTINUE                      00001940
C...
      UNPACK LABELS...              00001950
C...
      CALL UNPK(IJ,NN,MIJ,NOCC,NVIRT) 00001960
      CALL UNPK(JK,MM,MJK,NOCC,NVIRT) 00001970
C...
      SUM OVER J AND A FOR DIAGRAM A 00001980
C...
      DO 4 IB=1,NVIRT                00001990

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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
00002400
*** FIND <IJ/AB>, <IJ/BA>, <JK/DA>, <JK/AD> 00002410
*** I1=MIJ(IA,IB)      00002420
I2=MIJ(IB,IA)        00002430
J1=MIJ(IA,IO)        00002440
J2=MIJ(IO,IA)        00002450
K1=MJK(ID,IA)        00002460
K2=MJK(IA,IO)        00002470
L1=MJK(IB,IA)        00002480
L2=MJK(IA,IB)        00002490
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(I1.GE.J1) 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(J1.GE.K1) 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
00002870
IF(LIK) GOTO 23       00002880
IF(LJK.OK.LA3) GOTO 21 00002890
IF(LIJ.OK.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
IF(LIJ.OR.LAD) GOTO 22    00003010
TD1=S2*Q2/DJKAB          00003020
TD2=S2*(Q1-Q2)/DJKAB     00003030
TD3=S1*Q1/DJKAB          00003040
GOTO 24                  00003050
22 CONTINUE
TD1=S2*Q2/DJKAB          00003060
TD2=2                     00003070
TD3=S1*Q1/DJKAB          00003080
24 CONTINUE
23 CONTINUE
IF(LJK.OR.LAB) GOTO 25    00003090
IF(LIJ.OR.LAB) GOTO 26    00003100
TB1=((P1-P2)*(R1-R2)+P2*R2)/DIJAB 00003110
TB2=((P1-P2)*R2+P2*(R1-R2))/DIJAB 00003120
TB3=P1*R1/DIJAB          00003130
GOTO 27                  00003140
26 CONTINUE
TB1=P2*R2/DIJAB          00003150
TB2=P2*(R1-R2)/DIJAB     00003160
TB3=P1*R1/DIJAB          00003170
GOTO 27                  00003180
25 CONTINUE
IF(LIJ.OR.LAB) GOTO 28    00003190
TB1=P2*R2/DIJAB          00003200
TB2=(P1-P2)*R2/DIJAB     00003210
TB3=P1*R1/DIJAB          00003220
GOTO 27                  00003230
28 CONTINUE
TB1=P2*R2/DIJAB          00003240
TB2=2                     00003250
TB3=P1*R1/DIJAB          00003260
27 CONTINUE
C...
TA1=TB1/DJKAD            00003270
TA2=TB2/DJKAD            00003280
TA3=TB3/DJKAD            00003290
TA(1)=TA(1)+TA1          00003300
TA(2)=TA(2)+TA2          00003310
TA(3)=TA(3)+TA3          00003320
TB(1)=TB(1)+TB1          00003330
TB(2)=TB(2)+TB2          00003340
TB(3)=TB(3)+TB3          00003350
IF(LIK) GOTO 6            00003360
TD(1)=TD(1)+TD1          00003370
TD(2)=TD(2)+TD2          00003380
TD(3)=TD(3)+TD3          00003390
6 CONTINUE
DO 8 IS=1,3                00003400
FA(IB>ID,IS)=TA(IS)+FA(IB>ID,IS) 00003410
GA(IB>ID,IS)=TB(IS)+GA(IB>ID,IS) 00003420
IF(LIK) GOTO 8            00003430
GB(IB>ID,IS)=TD(IS)+GB(IB>ID,IS) 00003440
8 CONTINUE
5 CONTINUE
4 CONTINUE
C...
SUM OVER A AND B FOR DIAGRAMS F+G 00003450
C...
DO 50 IA=1,NVIRT           00003460
IIA=IA+NOCC                00003470
DO 51 IB=1,NVIRT           00003480
LAB=(IA.EQ.IB)              00003490
IIB=IB+NOCC                00003500
EAB=E(IIA)+E(IIB)          00003510
DIJAB=EIJ-EAB              00003520
DJKAB=EJK-EAB              00003530
C...
FIND <IJ/AB>, <IJ/BA>, <JK/AB>, <JK/BA> 00003540
C... 00003550
00003560
00003570
00003580
00003590
00003600
00003610
00003620
00003630
00003640
00003650
00003660
00003670
00003680
00003690
00003700
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(I1.GE.J1) GOTO 52 00003780
ISAVE=I1
I1=I2
I2=ISAVE
52 CONTINUE
IF(J1.GE.K) GOTO 53 00003820
ISAVE=J1
J1=J2
J2=ISAVE
53 CONTINUE
P1=Z                   00003830
P2=Z                   00003840
Q1=Z                   00003850
Q2=Z                   00003860
IF(I1.NE.0) P1=VIJ(I1) 00003870
IF(I2.NE.0) P2=VIJ(I2) 00003880
IF(J1.NE.0) Q1=VJK(J1) 00003890
IF(J2.NE.0) Q2=VJK(J2) 00003900
00003910
IF(LIJ.OR.LJK.OR.LAB) GOTO 30 00003920
T=(P1-P2)*(Q1-Q2)+P1*Q1+P2*Q2 00003930
TIK=TIK+T/DIJAB          00003940
IF(LIK) GOTO 31          00003950
TKI=TKI+T/DJKAB          00003960
31 CONTINUE
SIK=SIK+T/(DJKAB*DIJAB) 00004020
GOTO 32
30 CONTINUE
T=P1*Q1+P2*Q2          00004030
TIK=TIK+T/DIJAB          00004040
IF(LIK) GOTO 33          00004050
TKI=TKI+T/DJKAB          00004060
33 CONTINUE
SIK=SIK+T/(DJKAB*DIJAB) 00004110
32 CONTINUE
51 CONTINUE
50 CONTINUE
00004120
00004130
00004140
00004150
00004160
00004170
00004180
00004190
00004200
00004210
00004220
00004230
00004240
00004250
00004260
00004270
00004280
00004290
00004300
00004310
00004320
00004330
00004340
00004350
00004360
00004370
00004380
00004390
00004400
00004410
00004420
00004430
00004440
00004450
00004460
*** COMPLETE EVALUATION OF DIAGRAM A
DO 9 IB=1,NVIRT          00004200
DO 10 ID=1,NVIRT          00004210
DO 11 IS=1,3              00004220
VA=FA(IB, ID, IS)*GA(IB, ID, IS)+VA 00004230
IF(LIK) GOTO 11          00004240
VA=FA(ID, IS, IS)*GB(IB, ID, IS)+VA 00004250
11 CONTINUE
10 CONTINUE
9 CONTINUE
00004260
00004270
00004280
00004290
00004300
00004310
00004320
00004330
00004340
00004350
00004360
00004370
00004380
00004390
00004400
00004410
00004420
00004430
00004440
00004450
00004460
*** COMPLETE EVALUATION OF DIAGRAMS F+G
2 VB=SIK*(TIK+TKI)+VB 00004330
1 CONTINUE
00004340
00004350
00004360
00004370
00004380
00004390
00004400
00004410
00004420
00004430
00004440
00004450
00004460
1001 WRITE(6,1001)
1001 FORMAT(//, 'EVALUATION OF DIAGRAMS A, F+G COMPLETED')
00004470
*** RETURN
END
SUBROUTINE QU4B(E,NOCC,NVIRT,NT,VA,VB,VIJ,MIJ,VKL,MKL,
& GDE,FDE,NIJ,NKL,IJ,KL,NV)
00004480
00004490
00004500
00004510
00004520
00004530
00004540
00004550
00004560
00004570
00004580
00004590
00004600
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*** PROGRAMS TO EVALUATE 4-TH ORDER ENERGY DIAGRAMS INVOLVING

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C... QUADRUPLY-EXCITED STATES.          00004470
C... THIS SUBROUTINE EVALUATES DIAGRAMS B+C, D+E 00004480
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C...                                             00005200
C...                                             00005210

IMPLICIT REAL*8 (A-H,O-Z)           00004510
DIMENSION E(1),FBC(3),GBC(3),FDE(NVIRT,NVIRT),GDE(NVIRT,NVIRT), 00004520
&MIJ(NVIRT,NVIRT),MKL(NVIRT,NVIRT) 00004530
DIMENSION VIJ(NV),VKL(NV)           00004540
LOGICAL*LIJ,LJL,LIK,LKL,LAC,LAB,LBC 00004550
DIMENSION NIJ(1),NKL(1)             00004560
INTEGER IJ(NV),KL(NV)               00004570
DIMENSION DUMMY(10)                 00004580
DATA Z/0.0D+00/                      00004590

C... WRITE(6,1000)                   00004600
1000 FORMAT(//' BEGIN EVALUATION OF DIAGRAMS B+C, D+E') 00004610
C... VA=Z                           00004620
C... VB=Z                           00004630
C... FDE, GDE :: INTERMEDIATES FOR DIAGRAMS D+E 00004640
C... DO 5 IA=1,NVIRT                00004650
C...   DO 5 IC=1,NVIRT              00004660
C...     FDE(IA,IC)=Z               00004670
C...     GDE(IA,IC)=Z               00004680
C...   5 CONTINUE                     00004690
C...   DO 1 I=1,NOCC                00004700
C...     DO 1 J=1,I                  00004710
C...       LIJ=(I.EQ.J)              00004720
C...     READ (IJ) BLOCK OF INTEGRALS 00004730
C...     READ(NT) II,JJ,NN            00004740
C...     NNN=NN+NN                  00004750
C...     CALL RFST(IJ,NN,NT)         00004760
C...     CALL RFST(NIJ,NNN,NT)        00004770
C...     REWIND NT                   00004780
C...     READ(NT) DUMMY             00004790
C...     CALL UNPK(IJ,NN,MIJ,NOCC,NVIRT) 00004800
C...     EIJ=E(I)+E(J)              00004810
C...   DO 2 K=1,I                   00004820
C...     LIK=(I.EQ.K)               00004830
C...     DO 2 L=1,K                 00004840
C...       LJL=(J.EQ.L)              00004850
C...       LKL=(K.EQ.L)              00004860
C...       IF(LIK.AND.L.GT.J) GOTO 2 00004870
C...     READ (KL) BLOCK OF INTEGRALS 00004880
C...     READ(NT) KK,LL,MM            00004890
C...     MMM=MM+MM                  00004900
C...     CALL RFST(KL,MM,NT)         00004910
C...     CALL RFST(NKL,MMM,NT)        00004920
C...     CALL UNPK(KL,MM,MKL,NOCC,NVIRT) 00004930
C...     EKL=E(K)+E(L)              00004940
C... SUM OVER A AND B FOR DIAGRAMS B+C 00004950
C... F1=Z                           00004960
C... F2=Z                           00004970
C... F3=Z                           00004980
C... GA1=Z                          00004990
C... GA2=Z                          00005000
C... GA3=Z                          00005010
C... GB1=Z                          00005020

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

```

```

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

```


