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COMMUTE-A Computer Code for Noncommutative Algebra

LAURENCE S. ROTHMAN

5 July 1979

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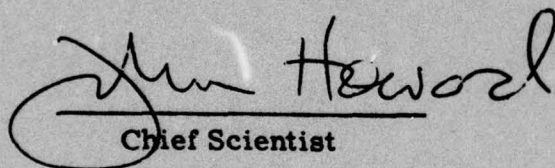


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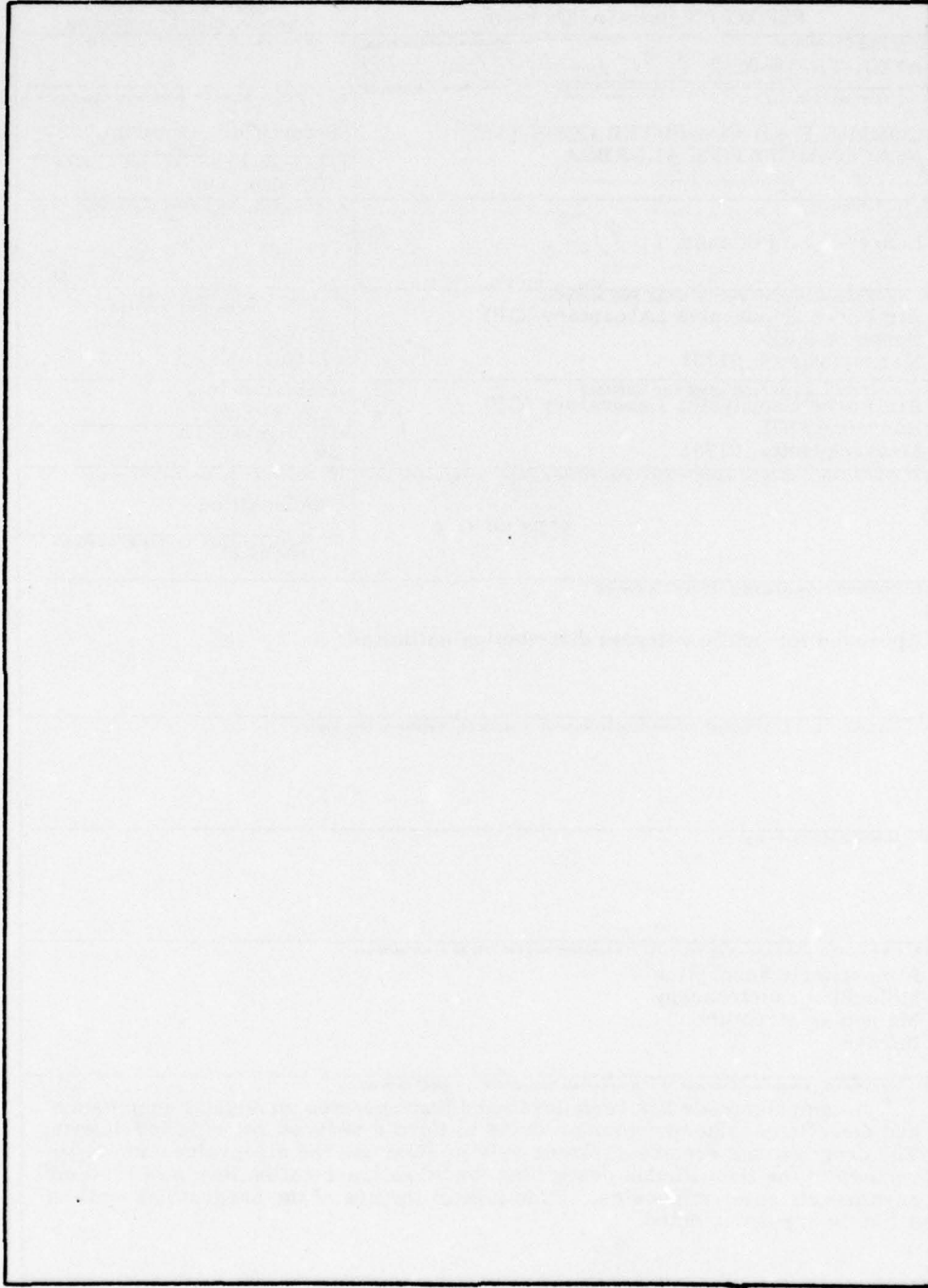
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Preface

I wish to acknowledge the many contributions and developmental efforts of S. A. Clough to the problems represented in this report and to the helpful discussions we have had.

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COMMUTE – A Computer Code for Noncommutative Algebra

1. INTRODUCTION

In the course of investigations of infrared absorbing frequencies and line strengths of triatomic molecules of atmospheric interest, the main theoretical approach has invariably involved the necessity of calculating complex commutators of quantum operators. In particular, when dealing with the vibration-rotation Hamiltonian, one encounters commutators and anticommutators of angular momentum operators and related direction cosine operators between molecular-fixed axes and space-fixed axes. This report presents a computerized method of generating simplified series of operators, a so-called reduced set, from given initial commutators, anticommutators, or general operator polynomials. This computer program, which implements noncommutative algebra, is called COMMUTE.

2. THEORY

2.1 General Formulation

The general problem is one in which there is a commutator consisting of products of some fundamental operators, whose basic commutation relation is

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given. Through successive application of this fundamental commutation relation, the original commutator can be simplified into a series of anticommutators. This can be expressed symbolically as

$$C_0 [\underline{Q}'_0, \underline{Q}''_0] = C_1 \{ \underline{Q}'_1, \underline{Q}''_1 \} + C_2 \{ \underline{Q}'_2, \underline{Q}''_2 \} + \dots + C_i \{ \underline{Q}'_i, \underline{Q}''_i \} + \dots \quad (1)$$

where the \underline{Q}'_i and \underline{Q}''_i are, in general, products of operators, the C_i are either pure real or pure imaginary numbers, and the brackets and braces are the standard notation for commutators and anticommutators, that is,

$$[\underline{A}, \underline{B}] = \underline{A}\underline{B} - \underline{B}\underline{A}$$

and

$$\{ \underline{A}, \underline{B} \} = \underline{A}\underline{B} + \underline{B}\underline{A} \quad (2)$$

The series in Eq. (1) in practice terminates rapidly; the number of terms is proportional to the degree of the original operators \underline{Q}'_0 and \underline{Q}''_0 . The degree, that is, the sum of the powers of fundamental operators in the operator polynomial on the right side of Eq. (1), is at least one less than the original operator polynomial $[\underline{Q}'_0, \underline{Q}''_0]$. In fact, if the original commutator is of degree n , then the series will contain terms of degree $n-1$, $n-3$, $n-5$, etc. (Of course, terms may be missing altogether if their coefficients, C_i , are identically zero.) Furthermore, it follows from the preservation of hermiticity (or antihermiticity) that if C_0 is an imaginary number, then the coefficients of the anticommutators are all pure real. Conversely, if C_0 is real, the coefficients on the right side of Eq. (1) are pure imaginary.

These remarks will be demonstrated in the examples that follow.

2.2 Diagonalizing the Hamiltonian

The problem discussed in this section has been presented by Rothman and Clough¹ and typifies the use of program COMMUTE. A contact transformation

$$e^{i\underline{S}'} \underline{H} e^{-i\underline{S}'} \quad (3)$$

is applied to the Hamiltonian to yield a transformed Hamiltonian expanded in a Taylor's series

1. Rothman, L.S. and Clough, S.A. (1971) J. Chem. Phys. 55:504.

$$\underline{H}'(\lambda) = \underline{H} + \sum_{n=1}^{\infty} \frac{\lambda^n i^n}{n!} [\underline{S}', \dots [\underline{S}', [\underline{S}', \underline{H}] \dots] \dots] \quad (4)$$

where λ is an expansion parameter and \underline{S}' is an Hermitian operator ($i = \sqrt{-1}$). Utilizing the order of magnitude arguments given in Reference 1, one arrives at expressions for the "rotational Hamiltonian", Eqs. (31) of Reference 1. \underline{S}' is chosen to remove certain off-diagonal terms in the Hamiltonian and, as such, is itself formed of angular momentum operators. Thus, expressions for the rotational Hamiltonian contain numerous commutators of angular momentum operators. In Appendix B. 1, two representative commutators arising from the contact transformation are given.

An alternative scheme for calculating the rotational commutators has been presented in the work of Amat et al.² In their approach, the contribution of a chosen operator term is given as a function of commutators of various directions. As such, their procedure is the inverse of the one discussed here.

2.3 Reducing Operations

The rotational Hamiltonian through fourth order of a planar molecule in the XZ plane is of the form

$$\begin{aligned} \underline{H}^{\dagger\dagger} = & h_v + A \underline{P}_z^2 + B \underline{P}_x^2 + C \underline{P}_y^2 + D \{ \underline{P}_x, \underline{P}_z \} + \sum_{\alpha\beta\gamma\delta} \rho'_{\alpha\beta\gamma\delta} \underline{P}_\alpha \underline{P}_\beta \underline{P}_\gamma \underline{P}_\delta \\ & + \sum_{\alpha\beta\gamma\delta\epsilon\eta} \Phi'_{\alpha\beta\gamma\delta\epsilon\eta} \underline{P}_\alpha \underline{P}_\beta \underline{P}_\gamma \underline{P}_\delta \underline{P}_\epsilon \underline{P}_\eta \quad (5) \end{aligned}$$

where h_v represents the vibrational contribution to the Hamiltonian; A, B, C, and D are coefficients of the quadratic terms in the angular momentum; the $\rho'_{\alpha\beta\gamma\delta}$ are coefficients of the quartic terms in angular momentum; and the $\Phi'_{\alpha\beta\gamma\delta\epsilon\eta}$ are coefficients of the sextic terms in angular momentum. For the case of orthorhombic symmetry, there are 15 nonvanishing $\rho'_{\alpha\beta\gamma\delta}$ and 105 $\Phi'_{\alpha\beta\gamma\delta\epsilon\eta}$. A great amount of the simplification can be obtained in the Hamiltonian by application of the commutation relations of angular momentum to these coefficients. The

2. Amat, G., Goldsmith, M., and Nielsen, H.H. (1957) J. Chem. Phys. 27:838.

resulting reduced form of $\underline{H}^{\dagger\dagger}$ for asymmetric rotors of orthorhombic symmetry thus contains only 19 coefficients (Kneizys et al³):

$$\begin{aligned} \underline{H}^{\dagger\dagger} = & h_v + A \underline{P}_z^2 + B \underline{P}_x^2 + C \underline{P}_y^2 \\ & + T_1 \underline{P}_x^4 + T_2 \underline{P}_y^4 + T_3 \underline{P}_z^4 \\ & + T_4 \{ \underline{P}_y^2, \underline{P}_z^2 \} + T_5 \{ \underline{P}_x^2, \underline{P}_z^2 \} + T_6 \{ \underline{P}_x^2, \underline{P}_y^2 \} \\ & + \Phi_1 \underline{P}_x^6 + \Phi_2 \underline{P}_y^6 + \Phi_3 \underline{P}_z^6 + \Phi_4 \{ \underline{P}_x^2, \underline{P}_y^4 \} \\ & + \Phi_5 \{ \underline{P}_y^2, \underline{P}_x^4 \} + \Phi_6 \{ \underline{P}_y^2, \underline{P}_z^4 \} + \Phi_7 \{ \underline{P}_z^2, \underline{P}_y^4 \} \\ & + \Phi_8 \{ \underline{P}_z^2, \underline{P}_x^4 \} + \Phi_9 \{ \underline{P}_x^2, \underline{P}_z^4 \} + \Phi_{10} (\underline{P}_x^2 \underline{P}_y^2 \underline{P}_z^2 + \underline{P}_z^2 \underline{P}_y^2 \underline{P}_x^2) . \end{aligned} \quad (6)$$

2.4 Minimal Set of Operators

It has been shown by Watson⁴ that the coefficients of the Hamiltonian of Eq. (6) are not all linearly independent for an asymmetric-top molecule. This gives rise to highly correlated coefficients when an attempt is made to estimate the coefficients in conjunction with a least squares approach with the experimental data (Flaud and Camy-Peyret,⁵ Rothman and Clough⁶). The indeterminacy can be further removed by successive unitary transformations on $\underline{H}^{\dagger\dagger}$ of the form

$$\underline{H}_w = e^{i\underline{S}} \underline{H}^{\dagger\dagger} e^{-i\underline{S}} . \quad (7)$$

Successive transformations of this type again lead to a series of commutators analogous to Eq. (4). The choice of elements s_{pqr} , where

$$\underline{S} = \sum_{pqr} s_{pqr} (\underline{P}_x^p \underline{P}_y^q \underline{P}_z^r + \underline{P}_z^r \underline{P}_y^q \underline{P}_x^p) , \quad (8)$$

3. Kneizys, F.X., Freedman, J.N., and Clough, S.A. (1966) J. Chem. Phys. 44:2552.

4. Watson, J.K.G. (1967) J. Chem. Phys. 46:1935; (1968) J. Chem. Phys. 48:4517.

5. Flaud, J.-M. and Camy-Peyret, C. (1973) Mol. Phys. 26:811.

6. Rothman, L.S. and Clough, S.A. (1975) Determination of Valence Force Constants for Water from Vibrational Data, Paper Presented at the Thirtieth Symposium on Molecular Structure and Spectroscopy, Ohio State University, Columbus, OH.

is arbitrary and can be made to reduce the Hamiltonian $\underline{H}^{\dagger\dagger}$ to contain only $(n + 1)$ independent terms of total degree n in the components of total angular momentum for each even value of n . The standard choice is to remove the coefficients of operators such that the matrix elements in the symmetric-top basis satisfy the selection rule $\Delta K = 0, \pm 2$, that is, the reduced Hamiltonian matrix in a given vibrational state is at worst tridiagonal (Yallabandi and Parker,⁷ Benedict et al⁸). This leads to the Watson reduced Hamiltonian

$$\begin{aligned} \underline{H}_w = & h_{000} + h_{100} \underline{P}^2 + h_{010} \underline{P}_z^2 + h_{001} (\underline{P}_x^2 - \underline{P}_y^2) \\ & + h_{200} \underline{P}^4 + h_{110} \underline{P}^2 \underline{P}_z^2 + h_{020} \underline{P}_z^4 + h_{101} \{ \underline{P}_z^2 (\underline{P}_x^2 - \underline{P}_y^2) \} \\ & + h_{011} \{ \underline{P}_z^2 (\underline{P}_x^2 - \underline{P}_y^2) \} + h_{300} \underline{P}^6 + h_{210} \underline{P}^4 \underline{P}_z^2 \\ & + h_{120} \underline{P}^2 \underline{P}_z^4 + h_{030} \underline{P}_z^6 + h_{201} \{ \underline{P}_z^4 (\underline{P}_x^2 - \underline{P}_y^2) \} \\ & + h_{111} \{ \underline{P}_z^2 \underline{P}_z^2 (\underline{P}_x^2 - \underline{P}_y^2) \} + h_{021} \{ \underline{P}_z^4 (\underline{P}_x^2 - \underline{P}_y^2) \} . \end{aligned} \quad (9)$$

Eq. (9) is given through fourth order, although many terms of high order in angular momentum can be preserved in the transformation Eq. (7) so that the equality is preserved. Notice that the choice of the parameters s_{pqr} has been made to eliminate any powers of the operator $(\underline{P}_x^2 - \underline{P}_y^2)$ greater than unity.

2.5 Direction Cosine Operators

Another example of the use of the commutator reduction is seen in the calculation of the dipole moment expansion (Clough et al,⁹ Flaud et al¹⁰). This problem requires the calculation of commutators of the type

$$[(\underline{P}_x^p \underline{P}_y^q \underline{P}_z^r + \underline{P}_z^r \underline{P}_y^q \underline{P}_x^p), \underline{\Phi}_\alpha] , \quad (10)$$

where the indices p, q, r are powers of angular momentum, and $\underline{\Phi}_\alpha$ is the direction cosine between the α -molecular-fixed axis and the space-fixed axis. The computer code COMMUTE generates series of reduced operators for the general

7. Yallabandi, K. Y. and Parker, P. M. (1968) J. Chem. Phys. 49:410.
8. Benedict, W. S., Clough, S. A., Frenkel, L., and Sullivan, T. E. (1970) J. Chem. Phys. 53:2565.
9. Clough, S. A., Beers, Y., Klein, G. P., and Rothman, L. S. (1973) J. Chem. Phys. 59:2254.
10. Flaud, J. -M., Camy-Peyret, C., Mandin, J. -Y., and Guelachvili, G. (1977) Mol. Phys. 34:413.

term (10) in a fashion similar to the results from the previous examples. The most general form of commutation operations involving the direction cosine operators occurs when performing a Watson-type transformation on the dipole moment expansion. The form of the commutator is then

$$[(P_x^p P_y^q P_z^r + P_z^r P_y^q P_x^p) , (P_x^s P_y^t P_z^u \Phi_\alpha + \Phi_\alpha P_z^u P_y^t P_x^s)] \quad (11)$$

Examples of the application of COMMUTE to terms (10) and (11) are given in Appendix B. 4 and B. 5.

References

1. Rothman, L.S. and Clough, S.A. (1971) J. Chem. Phys. 55:504.
2. Amat, G., Goldsmith, M., and Nielsen, H.H. (1957) J. Chem. Phys. 27:838.
3. Kneizys, F.X., Freedman, J.N., and Clough, S.A. (1966) J. Chem. Phys. 44:2552.
4. Watson, J.K.G. (1967) J. Chem. Phys. 46:1935; (1968) J. Chem. Phys. 48:4517.
5. Flaud, J.-M. and Camy-Peyret, C. (1973) Mol. Phys. 26:811.
6. Rothman, L.S. and Clough, S.A. (1975) Determination of Valence Force Constants for Water from Vibrational Data, Paper Presented at the Thirtieth Symposium on Molecular Structure and Spectroscopy, Ohio State University, Columbus, OH.
7. Yallabandi, K.Y. and Parker, P.M. (1968) J. Chem. Phys. 49:410.
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10. Flaud, J.-M., Camy-Peyret, C., Mandin, J.-Y., and Guelachvili, G. (1977) Mol. Phys. 34:413.

Appendix A

The Code COMMUTE

Provided in this Appendix is a complete listing of the program COMMUTE. Fundamental commutation relations are built in for the angular momentum operators and direction cosine operators. To distinguish the two types of operators, a general 6-vector was chosen with the correspondence: $U \rightarrow \Phi_x$, $V \rightarrow \Phi_y$, $W \rightarrow \Phi_z$, $X \rightarrow P_x$, $Y \rightarrow P_y$, and $Z \rightarrow P_z$.

The first input card indicates the number of terms in the initial polynomial that is to be reduced. However, the program automatically takes each initial term and forms an anticyclic pair to it. Thus, for the commutator $[P_x, P_y] = P_x P_y - P_y P_x$, it is only necessary to consider one term $P_x P_y$. The operator polynomial $[(P_x, P_z), P_y]$ should be considered as two terms for the program, $P_x P_z P_y$ and $P_z P_x P_y$; anticommutators should be expanded. This feature of doubling terms was undertaken since the primary use of the program requires commutator or anticommutator reduction. Single terms can nevertheless be handled as can be seen from the example in Appendix B. There is also the option on the first input card to allow the program to drive the reduction in a cyclic, that is, UVWXYZ, or anticyclic direction (ZYXWVU), thereby facilitating tests for axis invariance.

The second group of input cards (equal to the number of initial terms) indicates the number of operators, the coefficients, and the directions and exponents of the operators. The sample data deck accompanying the examples in Appendix B should suffice to explain the method of reading in the terms.

The program works on two "levels" at any time, a level being all terms of a given degree in exponent sum. The operators are scanned for their directions. If the directions are different, then the commutation relation is applied, if they are the same, then they are multiplied (exponents added). The action of the commutation relation creates a term at the next level. Terms at the second level are scanned for identical terms and cancelled when the coefficients are zero. When a level has been completely scanned and condensed, it is written as anti-commutators if the original term or terms was either hermitian or antihermitian. The process thus is one in which commutators are always "driven".

```

PROGRAM COMPUTE (INPUT, OUTPUT)                                COM 10
C                                                                COM 11
C          PROGRAM BY LAURENCE S. POTTMAN                      COM 12
C          OPTICAL PHYSICS DIVISION                            COM 13
C          AIR FORCE GEOPHYSICS LABORATORY                      COM 14
C          WEDFORD, MA 01731                                   COM 15
C                                                                COM 16
C THIS PROGRAM DERIVES TERMS CONTAINING ANGULAR MOMENTUM AND/OR COM 20
C DIRECTION COSINE OPERATORS INTO EITHER CYCLIC OR ANTICYCLIC COM 21
C (ANTICOMMUTATORS) THROUGH THE USE OF COMMUTATION RELATIONS. COM 22
C                                                                COM 25
C FOR THE ARRAYS IN PLANK COMMON:                               COM 30
C FIRST INDEX DESIGNATES LEVEL, SECOND TERM, THIRD POSITION OF OPERATOR. COM 40
C IFCSMAX(LEV,ITERM) = NUMBER OF OPERATORS IN ITERM.          COM 50
C ITERMPL(LEV) = TOTAL NUMBER OF TERMS IN LEV.                 COM 60
C PROGRAM WILL TERMINATE IF IT ENCOUNTERS: (1) TWELVE OR MORE OPERATORS COM 70
C IN A TERM, OR (2) 200 OR MORE TERMS AT A PARTICULAR LEVEL. COM 80
C                                                                COM 90
COMMON ITRM(2,199,11), IEXP(2,199,11), COEFF(2,199), IFCSMAX(2,199) COM 100
DIMENSION ITERMPL(2), DIR(6), X(11), X2(11), EPS(6,6), ICTEL(6,6), COM 110
IEXP(11), ICTIC(6), HEXF2(11), EPSVEC(36), ICVEC(36)           COM 120
DATA (CIP(I),I=1,6)/1HU,1HV,1HW,1HX,1HY,1HZ/                   COM 130
DATA (NDIG(I),I=1,9)/1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9/    COM 140
DATA HP,HLP,HFP,HPL,HMT,HR/1HF,1HG,1H,1H+,1H-,1H /            COM 150
C                                                                COM 160
C COMMUTATION RELATIONS:                                       COM 170
C                                                                COM 180
DATA EPSVEC/
C          U          V          W          X          Y          Z
U          0. ,      0. ,      0. ,      0. ,      -1. ,      1. ,
V          0. ,      0. ,      0. ,      1. ,      0. ,      -1. ,
W          0. ,      0. ,      0. ,      -1. ,      1. ,      0. ,
Y          0. ,      -1. ,      1. ,      0. ,      -1. ,      1. ,
Y          1. ,      0. ,      -1. ,      1. ,      0. ,      -1. ,
Z          -1. ,      1. ,      0. ,      -1. ,      1. ,      0. /

DATA ICVEC/
C          U          V          W          X          Y          Z
U          0 ,      0 ,      0 ,      0 ,      3 ,      2 ,
V          0 ,      0 ,      0 ,      3 ,      0 ,      1 ,
W          0 ,      0 ,      0 ,      2 ,      1 ,      0 ,
X          0 ,      2 ,      0 ,      0 ,      6 ,      5 ,
Y          3 ,      0 ,      1 ,      6 ,      0 ,      4 ,
Z          2 ,      1 ,      0 ,      5 ,      4 ,      0 /

DO 10 I=1,6
DO 10 J=1,6
IND=J+6*(I-1)
EPS(I,J)=EPSVEC(IND)
ICTEL(I,J)=ICVEC(IND)
10 CONTINUE
C                                                                COM 310
C                                                                COM 320
C (1) READ IN NUMBER OF INPUT TERMS (I2) AND WHETHER TERMS ARE TO BE COM 330
C ORTMEN (CYCLICALLY OR ANTICYCLICALLY (F6.1)):                COM 340
C (2) READ NUMBER OF OPERATORS (I2), COEFFICIENTS (2F6.1), AND DIRECTION COM 350
C AND EXPONENT OF EACH OPERATOR -- FORMAT (I2,2F6.1,11(1X,F1,I2,2X))! COM 360
C                                                                COM 370

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      LEV=1                                COM 380
      LEV2=2                                COM 390
20    READ 900, ITERM1(1),CYCLE            COM 400
      CYC=10*CYCLIC                          COM 410
      IF (CYCLE .LT. -1.1) CYC=10*ANTICYCLIC COM 420
      ITERM1(1)=2*ITERM1(1)                  COM 430
      TTL=ITERM1(1)                          COM 440
      CALL SFCOIN (TIME)                      COM 450
      PRINT 905, TIME,CYC                    COM 460
      IF (TTL.EQ.0) STOP                      COM 470
      DO 60 IT=1,TTL,2                        COM 480
      READ 900, MAX,COEFF (1,IT),COEFF (1,IT+1),X(IP),IFXP (1,IT,IF),IP=1,CCM COM 490
      1MAX)                                COM 500
      IPOSMAX(1,IT)=IPOSMAX(1,IT+1)=MAX      COM 510
      DO 70 I=1,MAX                          COM 520
      DO 70 J=1,I                             COM 530
      IF (DIR(J).EQ.X(I)) IDIR(1,IT,I)=J     COM 540
30    CONTINUE                               COM 550
C                                            COM 560
C AUTOMATICALLY SYMMETRIZE INPUT TERMS:    COM 570
C                                            COM 580
      TSUM=0                                COM 590
      DO 40 I=1,MAX                          COM 600
      ISUM=ISUM+TEXT(1,IT,I)                 COM 610
      J=MAX+1-I                              COM 620
      IDIR(1,IT+1,I)=IDIR(1,IT,J)           COM 630
      TEXT(1,IT+1,I)=IFXP(1,IT,J)          COM 640
      NI=IFXP(1,IT,I)                       COM 650
      NJ=IFXP(1,IT+1,I)                    COM 660
      HEXP(I)=HDIR(NI)                      COM 670
      HEXP2(I)=HDIR(NJ)                    COM 680
40    X2(I)=X(J)                            COM 690
C                                            COM 700
C TEST FOR HERMITICITY, -1 FOR NON-HERMITIAN INPUT OPERATOR, COM 710
C 0 FOR HERMITIAN OPERATOR, +1 FOR ANTI-HERMITIAN OPERATOR: COM 720
C                                            COM 730
      IPAT=COEFF (1,IT+1)/COEFF (1,IT)+1.1  COM 740
      ICPAT=ISUM-2*(TSUM/2)                 COM 750
      IHERM=1                                COM 760
      IF ((IPAT.EQ.1).AND.(ICPAT.EQ.0)) IHERM=0 COM 770
      IF ((IPAT.EQ.0).AND.(ICPAT.EQ.2)) IHERM=0 COM 780
      IF (IPAT.EQ.1) IHERM=-1               COM 790
C                                            COM 800
C PRINT INPUT TERMS:                       COM 810
C                                            COM 820
      IF ((MAX.EQ.1).OR.(IHERM.EQ.-1)) GO TO 50 COM 830
      PRINT 940, (HEXP(IP),HP,IP=1,MAX),HB,HB,HP,(HEXP2(IF),HB,IF=1,MAX) COM 840
      XSIGN=HAT                               COM 850
      IF (IPAT.EQ.2) XSIGN=HPL                COM 860
      CALL FRAC (COEFF (1,IT),IC,ND)         COM 870
      IF (ND.EQ.0) PRINT 910, IC,HP,HLP,HP,(HP,HP,IF=1,MAX),HB,XSIGN, COM 880
      1(HP,HP,IF=1,MAX),HB,HPD              COM 890
      IF ((ND.GT.0).AND.(ND.LE.64)) PRINT 920, IC,ND,HB,HLP,HB,(HP,HP, COM 900
      1IP=1,MAX),HP,XSIGN,(HB,HP,IF=1,MAX),HP,HPF COM 910
      IF (ND.GT.64) PRINT 930, COEFF (1,IT),HB,HLP,HB,(HP,HP,IF=1,MAX),HBCOM 920
      1,XSIGN,HP,HP,IF=1,MAX),HP,HPD      COM 930
      PRINT 940, (Y(IF),HP,IF=1,MAX),HB,HP,HP,(Y2(IF),HP,IF=1,MAX) COM 940

```

50	GO TO 60	COM 950
	PRINT 940, (HFXP(IP),HB,IP=1,MAX)	COM 960
	C=COEFF(1,IT)+COEFF(1,IT+1)	COM 970
	CALL FRACT(C,IC,ND)	COM 980
	IF (ND.EQ.0) PRINT 910, IC,HR,HB,HB,(HF,HB,IP=1,MAX)	COM 990
	IF ((ND.GT.0).AND.(ND.LE.64)) PRINT 920, IC,ND,HB,HB,+B,(HP,HB,	COM 1000
	1IP=1,MAX)	COM 1010
	IF (NO.5T.F4) PRINT 930, C,HR,HB,HB,(HP,HB,IP=1,MAX)	COM 1020
	PRINT 940, (X(IP),HB,IP=1,MAX)	COM 1030
60	CONTINUE	COM 1040
	PRINT 950	COM 1050
	C	COM 1060
	C INDFX LEVELS, TERMS, AND TEST POSITION OF OPERATORS (SHIFT LEVELS TO	COM 1070
	C SAVE STORAGE):	COM 1080
	C	COM 1090
	L=0	COM 1100
70	L=L+1	COM 1110
	IF (L.F7.1) GO TO 90	COM 1120
	ITL=ITERML(LEV2)	COM 1130
	IF (ITL.EQ.0) GO TO 20	COM 1140
	ITERML(LEV)=ITL	COM 1150
	DO 80 IT=1,ITL	COM 1160
	COEFF(LEV,IT)=COEFF(LEV2,IT)	COM 1170
	MAX=IFOSMAX(LEV2,IT)	COM 1180
	IPOSMAX(LEV,IT)=MAX	COM 1190
	DO 60 IP=1,MAX	COM 1200
	IDIR(LEV,IT,IP)=IDIR(LEV2,IT,IP)	COM 1210
80	IEXP(LEV,IT,IP)=IEXP(LEV2,IT,IP)	COM 1220
90	ITERML(LEV2)=ITERM=ITERM2=0	COM 1230
100	ITERM=ITERM+1	COM 1240
	IF (ITERML(LEV).EQ.0) GO TO 70	COM 1250
	IF (ITERM.GT.ITERML(LEV)) GO TO 340	COM 1260
110	IFOS=0	COM 1270
120	IPOS=IPOS+1	COM 1280
	IF (IFOS.GE.IFOSMAX(LEV,ITERM)) GO TO 390	COM 1290
	N=IPOS+1	COM 1300
	IF (IDIR(LEV,ITERM,N).EQ.IDIR(LEV,ITERM,IPOS)) GO TO 130	COM 1310
	IF (CYCLE.LT.-0.1) GO TO 121	COM 1320
	IF (IDIR(LEV,ITERM,IPOS).GT.IDIR(LEV,ITERM,N)) GO TO 160	COM 1330
	GO TO 120	COM 1340
121	IF (IDIR(LEV,ITERM,IPOS).LT.IDIR(LEV,ITERM,N)) GO TO 160	COM 1350
	GO TO 120	COM 1360
	C	COM 1370
	C CONTRACT ADJACENT OPERATORS HAVING IDENTICAL DIRECTIONS, IN LEV1	COM 1380
	C	COM 1390
130	IEXP(LEV,ITERM,IPOS)=IEXP(LEV,ITERM,IPOS)+IEXP(LEV,ITERM,N)	COM 1400
	MAX=IFOSMAX(LEV,ITERM)-1	COM 1410
	IF (MAX.LT.N) GO TO 150	COM 1420
	GO 140 T=N,MAX	COM 1430
	IDIP(LEV,ITERM,I)=IDIR(LEV,ITERM,I+1)	COM 1440
140	IEXP(LEV,ITERM,I)=IEXP(LEV,ITERM,I+1)	COM 1450
150	IFOSMAX(LEV,ITERM)=MAX	COM 1460
	GO TO 110	COM 1470
	C	COM 1480
	C COMMUTE TWO OPERATORS IN LEV1	COM 1490
	C	COM 1500
160	IA=IDIP(LEV,ITERM,IPOS)	COM 1510

	I3=IDIR(LFV, ITERM, N)	COM 1520
	IEXP(LFV, ITERM, IPOS)=IEXP(LFV, ITERM, IPOS)-1	COM 1530
	IPOS MAX(LFV, ITERM)=IPOS MAX(LFV, ITERM)+2	COM 1540
	MAX=IPOS MAX(LFV, ITERM)	COM 1550
	IF (MAX.LT.1) GO TO 170	COM 1560
	PRINT 970, MAX, L, ITERM	COM 1570
	GO TO 20	COM 1580
170	LIM=MAX-N	COM 1590
	GO 180 T=1, LIM	COM 1600
	J=MAX+1-T	COM 1610
	IDIP(LFV, ITERM, J)=IDIP(LFV, ITERM, J-2)	COM 1620
180	IEXP(LFV, ITERM, J)=IEXP(LFV, ITERM, J-2)	COM 1630
	IEXP(LFV, ITERM, N+2)=IEXP(LFV, ITERM, N)-1	COM 1640
	IEXP(LFV, ITERM, N+1)=IEXP(LFV, ITERM, N)-1	COM 1650
	C	COM 1660
	C ELIMINATE ZERO-EXPONENTS IN LFV1	COM 1670
	C	COM 1680
	N2=N+2	COM 1690
	NGAM=N	COM 1700
	IF (IEXP(LFV, ITERM, N2).GT.0) GO TO 210	COM 1710
	MAX=IPOS MAX(LFV, ITERM)-1	COM 1720
	IF (MAX.LT.N2) GO TO 200	COM 1730
	GO 190 T=N2, MAX	COM 1740
	IDIP(LFV, ITERM, I)=IDIP(LFV, ITERM, I+1)	COM 1750
190	IEXP(LFV, ITERM, I)=IEXP(LFV, ITERM, I+1)	COM 1760
200	IPOS MAX(LFV, ITERM)=MAX	COM 1770
210	IF (IEXP(LFV, ITERM, IPOS).GT.0) GO TO 230	COM 1780
	NGAM=NGAM-1	COM 1790
	MAX=IPOS MAX(LFV, ITERM)-1	COM 1800
	GO 220 I=IPOS, MAX	COM 1810
	IDIP(LFV, ITERM, I)=IDIP(LFV, ITERM, I+1)	COM 1820
220	IEXP(LFV, ITERM, I)=IEXP(LFV, ITERM, I+1)	COM 1830
	IPOS MAX(LFV, ITERM)=MAX	COM 1840
230	IF (EPS(IA, IB).EQ.0.) GO TO 110	COM 1850
	C	COM 1860
	C CREATE TERM2 IN LFV2 (= LFV+1)	COM 1870
	C	COM 1880
	ITERM2=ITERM+1	COM 1890
	IF (ITERM2.LE.199) GO TO 240	COM 1900
	PRINT 980, ITERM2, L, ITERM	COM 1910
	GO TO 23	COM 1920
240	ITERM1(LFV2)=ITERM2	COM 1930
	IPOS MAX(LFV2, ITERM2)=IPOS MAX(LFV, ITERM)-1	COM 1940
	IF=NGAM-1	COM 1950
	IF (IF.LT.1) GO TO 260	COM 1960
	GO 250 T=1, IF	COM 1970
	IDIP(LFV2, ITERM2, I)=IDIP(LFV, ITERM, I)	COM 1980
250	IEXP(LFV2, ITERM2, I)=IEXP(LFV, ITERM, I)	COM 1990
260	COEFF(LFV2, ITERM2)=EPS(IA, IB)*COEFF(LFV, ITERM)	COM 2000
	IDIP(LFV2, ITERM2, NGAM)=ICTBL(IA, IB)	COM 2010
	IEXP(LFV2, ITERM2, NGAM)=1	COM 2020
	MAX=IPOS MAX(LFV2, ITERM2)	COM 2030
	N1=NGAM+1	COM 2040
	IF (MAX.LT.N1) GO TO 280	COM 2050
	GO 270 T=N1, MAX	COM 2060
	IDIP(LFV2, ITERM2, I)=IDIP(LFV, ITERM, I+1)	COM 2070
270	IEXP(LFV2, ITERM2, I)=IEXP(LFV, ITERM, I+1)	COM 2080

C		COM 2090
C	CONTRACT ADJACENT OPERATORS HAVING IDENTICAL DIRECTIONS IN LEV2:	COM 2100
C		COM 2110
280	IF (MAX.LT.2) GO TO 310	COM 2120
	LMAX=MAX	COM 2130
	LT=1	COM 2140
	DO 300 I=2,MAX	COM 2150
	LI=LI+1	COM 2160
	IF (LMAX.LT.LI) GO TO 310	COM 2170
	IF (IDIR(LEV2,ITERM2,LI).NE.IDIR(LEV2,ITERM2,LI-1)) GC TC 300	COM 2180
	IFXP(LEV2,ITERM2,LI-1)=IEXP(LEV2,ITERM2,LI-1)+IEXP(LEV2,ITERM2,LI)	COM 2190
	LMAX=LMAX-1	COM 2200
	IPOSMAX(LEV2,ITERM2)=LMAX	COM 2210
	IF (LMAX.LT.LI) GO TO 310	COM 2220
	DO 290 J=LI,LMAX	COM 2230
	IDIR(LEV2,ITERM2,J)=IDIR(LEV2,ITERM2,J+1)	COM 2240
290	JFYF(LEV2,ITERM2,J)=IEXP(LEV2,ITERM2,J+1)	COM 2250
	LI=LI-1	COM 2260
300	CONTINUE	COM 2270
C		COM 2280
C	ADD IDENTICAL TERMS IN LEV2:	COM 2290
C		COM 2300
310	IF (ITERM2.LE.1) GO TO 110	COM 2310
	MAX=IPOSMAX(LEV2,ITERM2)	COM 2320
	K=ITERM2-1	COM 2330
	DO 330 I=1,K	COM 2340
	IF (IPOSMAX(LEV2,I).NE.MAX) GO TO 330	COM 2350
	DO 320 J=1,MAX	COM 2360
	IF (IDIR(LEV2,I,J).NE.IDIR(LEV2,ITERM2,J)) GO TO 330	COM 2370
	IF (IFXP(LEV2,I,J).NE.IEXP(LEV2,ITERM2,J)) GO TO 330	COM 2380
320	CONTINUE	COM 2390
	COEFF(LEV2,I)=COEFF(LEV2,I)+COEFF(LEV2,ITERM2)	COM 2400
	ITERM2=ITERM2-1	COM 2410
	ITERML(LEV2)=ITERM2	COM 2420
	CALL CANCEL(LEV2,ITERM2,I,ITERML(LEV2))	COM 2430
	GC TO 110	COM 2440
330	CONTINUE	COM 2450
	GO TO 110	COM 2460
C		COM 2470
C	TEST FOR ANTI-COMMUTATORS OR COMMUTATORS:	COM 2480
C		COM 2490
340	IF (ITERM.FO.-1) GO TO 460	COM 2500
	ISUM=0	COM 2510
	MAX=IPOSMAX(LEV,1)	COM 2520
	DO 350 I=1,MAX	COM 2530
350	ISUM=ISUM+JFYF(LEV,1,I)	COM 2540
	IPAR=ISUM-2*(ISUM/2)	COM 2550
	IF (IPAR.FO.IPAR) GO TO 460	COM 2560
	ITL=ITERML(LEV)	COM 2570
	IF (ITL.LT.100) GO TO 360	COM 2580
	PRINT 999, ITL,L,ITERM	COM 2590
	GO TO 20	COM 2600
360	DO 380 IT=1,ITL	COM 2610
	MAX=IPOSMAX(LEV,IT)	COM 2620
	IPOSMAX(LEV,IT+ITL)=MAX	COM 2630
	COEFF(LEV,IT)=(.5*COEFF(LEV,IT)	COM 2640
	COEFF(LEV,IT+ITL)=-COEFF(LEV,IT)	COM 2650

	DO 370 I=1,MAX	COM 2660
	J=MAX+1-I	COM 2670
	IEXP(LFV,IT+ITL,J)=IEXP(LEV,IT,I)	COM 2680
370	IDIP(LEV,IT+ITL,J)=IDIR(LEV,IT,I)	COM 2690
380	CONTINUE	COM 2700
	ITERM=ITL+1	COM 2710
	ITERML(LEV)=2*ITL	COM 2720
	GO TO 110	COM 2730
C		COM 2740
C	ADD IDENTICAL TERMS IN LEV:	COM 2750
C		COM 2760
390	IF (ITERM.EQ.1) GO TO 440	COM 2770
	MAX=IPDSMAX(LEV,ITERM)	COM 2780
	K=ITERM-1	COM 2790
	DO 430 I=1,K	COM 2800
	IF (IPDSMAX(LFV,I).NE.MAX) GO TO 430	COM 2810
	DO 400 J=1,MAX	COM 2820
	IF (IDIR(LFV,I,J).NE.IDIR(LEV,ITERM,J)) GO TO 430	COM 2830
	IF (IFXP(LFV,I,J).NE.IFXP(LEV,ITERM,J)) GO TO 430	COM 2840
400	CONTINUE	COM 2850
	COEFF(LEV,J)=COEFF(LEV,I)+COEFF(LEV,ITERM)	COM 2860
	ITERML(LEV)=ITERML(LEV)-1	COM 2870
	ITL=ITERML(LEV)	COM 2880
	IF (ITL.LT.ITERM) GO TO 420	COM 2890
	DO 410 IT=ITERM,ITL	COM 2900
	LIM=IPDSMAX(LEV,IT+1)	COM 2910
	COEFF(LEV,IT)=COEFF(LEV,IT+1)	COM 2920
	IPDSMAX(LEV,IT)=LIM	COM 2930
	DO 410 IP=1,LIM	COM 2940
	IDIP(LEV,IT,IP)=IDIP(LEV,IT+1,IP)	COM 2950
410	IEXP(LEV,IT,IP)=IEXP(LEV,IT+1,IP)	COM 2960
420	ITERM=ITERM-1	COM 2970
	GO TO 450	COM 2980
430	CONTINUE	COM 2990
	GO TO 100	COM 3000
C		COM 3010
C	CANCEL ZERO-COEFFICIENT TERMS IN LEV:	COM 3020
C		COM 3030
440	I=1	COM 3040
450	CALL CANCEL (LFV,ITERM,I,ITERML(LEV))	COM 3050
	GO TO 100	COM 3060
C		COM 3070
C	WRITE ANSWERS:	COM 3080
C		COM 3090
460	ITL=ITERML(LEV)	COM 3100
	IF (ITL.EQ.0) GO TO 70	COM 3110
	IF (L.EQ.1) GO TO 470	COM 3120
	LL=L-1	COM 3130
	PRINT 950, LL	COM 3140
470	DO 500 IT=1,ITL	COM 3150
	IF (ABS(COEFF(LEV,IT)).LT.1.E-20) GO TO 500	COM 3160
	MAX=IPDSMAX(LEV,IT)	COM 3170
	DO 480 I=1,MAX	COM 3180
	J=MAX+1-I	COM 3190
	NI=IDIR(LEV,IT,I)	COM 3200
	X(I)=DIR(NJ)	COM 3210
	NII=IFXP(LEV,IT,I)	COM 3220

```

      HEXP(I)=40IG(NII)                                COM 3230
      X2(J)=X(I)                                        COM 3240
480   HEXP2(J)=HEXP(I)                                COM 3250
      IF ((MAX.EQ.1).OR.(IHERM.EQ.-1)) GO TO 490      COM 3260
      PRINT 940, (HEXP(IP),HB,IP=1,MAX),HB,HB,HE, (HEXP2(IP),HE,IP=1,MAX) COM 3270
      C=COEFF(LEV,IT)/2.                                COM 3280
      CALL FRACT (C,IC,ND)                              COM 3290
      IF (ND.EQ.0) PRINT 910, IC,HB,HLP,HB, (HP,HB,IP=1,MAX),HB,HFL, COM 3300
      1(HB,HP,IP=1,MAX),HB,HRP                          COM 3310
      IF ((ND.GT.0).AND.(ND.LE.64)) PRINT 920, IC,ND,HB,HLP,HB, (HP,HB, COM 3320
      1IP=1,MAX),HB,HPL, (HB,HP,IP=1,MAX),HB,HRP      COM 3330
      IF (ND.GT.64) PRINT 930, C,HB,HLP,HB, (HP,HB,IP=1,MAX),HB,HFL, COM 3340
      1(HB,HP,IP=1,MAX),HB,HRP                          COM 3350
      PRINT 940, (X(IP),HE,IP=1,MAX),HB,HB,HB, (Y2(IP),HB,IP=1,MAX) COM 3360
      GO TO 500                                          COM 3370
490   PRINT 940, (HEXP(IP),HB,IP=1,MAX)                COM 3380
      CALL FRACT (COEFF(LEV,IT),IC,ND)                COM 3390
      IF (ND.EQ.0) PRINT 910, IC,HP,HB,HB, (HP,HP,IP=1,MAX) COM 3400
      IF ((ND.GT.0).AND.(ND.LE.64)) PRINT 920, IC,ND,HB,HB,HB, (HP,HB, COM 3410
      1IP=1,MAX)                                        COM 3420
      IF (ND.GT.64) PRINT 930, COEFF(LEV,IT),HB,HE,HB, (HP,HE,IP=1,MAX) COM 3430
      PRINT 940, (X(IP),HB,IP=1,MAX)                  COM 3440
500   CONTINUE                                         COM 3450
      GO TO 70                                          COM 3460
C
900   FORMAT (T2,2F6.1,11(1X,A1,I2,2Y))              COM 3480
905   FORMAT (30F1 ***** THE TIME IS NOW =,F9.3,19H SECONDS ***** COM 3490
      1***5X,A10/)
910   FORMAT (14Y,IF,80A1)                            COM 3510
920   FORMAT (11Y,IF,"/",I2,80A1)                   COM 3520
930   FORMAT (17Y,F12.6,80A1)                        COM 3530
940   FORMAT (26Y,80A1)                              COM 3540
950   FORMAT (140,24X"EQUALS"/)                      COM 3550
960   FORMAT (140/140,24X,I2/23X,54+IY */)          COM 3560
970   FORMAT (" PROFITED:IFOSMAX(LEV, ITERM)=" ,3I6) COM 3570
980   FORMAT (" PROFITED:ITERM2=" ,3I6)              COM 3580
990   FORMAT (" PROFITED:ITERML(LEV)=" ,3I6)         COM 3590
      END                                              COM 3600

```

	SUBROUTINE CANCEL (L,ITERM,ITE,ITL)	CAN 10
	C THIS SUBROUTINE	CAN 14
	C ANNHILATES A TERM WHOSE COEFFICIENT IS LESS THAN 1.E-12.	CAN 15
	COMMON IDIF(2,199,11),IEXP(2,199,11),COEFF(2,199),IFOSMAX(2,199)	CAN 20
	IF (ABS(COEFF(L,ITE)).GT.1.E-12) RETURN	CAN 30
	ITERM=ITERM-1	CAN 40
	ITL=ITL-1	CAN 50
	IF (ITL.LT.ITF) RETURN	CAN 60
	DO 10 IT=ITE,ITL	CAN 70
	MAX=IFOSMAX(L,IT+1)	CAN 80
	COEFF(L,IT)=COEFF(L,IT+1)	CAN 90
	IFOSMAX(L,IT)=MAX	CAN 100
	DO 10 IP=1,MAX	CAN 110
	IDIF(L,IT,IP)=IDIF(L,IT+1,IP)	CAN 120
10	IEXP(L,IT,IP)=IEXP(L,IT+1,IP)	CAN 130
	RETURN	CAN 140
	END	CAN 150-

	SUBROUTINE FRACT (C,IC,ND)	FRA 10
	C THIS SUBROUTINE ATTEMPTS TO WRITE COEFFICIENTS AS INTEGERS, OR	FRA 15
	C FRACTIONS IF THEY ARE AT LEAST MULTIPLES OF 1/64.	FRA 20
	ND=C	FRA 30
	YC=C+SIGN(1.E-08,C)	FRA 40
	IC=YC	FRA 50
	DIFCO=ABS(YC-FLOAT(IC))	FRA 60
	IF (DIFCO.LT.1.E-06) RETURN	FRA 70
	DO 10 I=1,7	FRA 80
	ND=2**I	FRA 90
	DIF=FLOAT(ND)*DIFCO	FRA 100
	IDIF=ND+1.E-08	FRA 110
	IF (DIF-FLOAT(IDIF)).LT.1.E-06) GO TO 20	FRA 120
10	CONTINUE	FRA 130
	RETURN	FRA 140
20	IC=ND*IC+TSIGN(IDIF,IC)	FRA 150
	RETURN	FRA 160-
	END	

Appendix B

EXAMPLES

B.1 COMMUTATORS ARISING FROM DIAGONALIZATION OF HAMILTONIAN

$$[\{P_x, P_z\}, P_y^2]$$

Input cards:

```

2
3  0.5  -0.5 X 1  Z 1  Y 2
3  0.5  -0.5 Z 1  X 1  Y 2
    
```

Result:

```

      1 1 2      2 1 1
1/ 2 ( P P P - P P P )
      X Z Y      Y Z Y
      1 1 2      2 1 1
1/ 2 ( P P P - P P P )
      Z X Y      Y X Z
    
```

EQUALS

```

      1
+IM *
      2 1      1 2
1 ( P P + P P )
      X Y      Y X
      1 2      2 1
-1 ( P P + P P )
      Y Z      Z Y
    
```

$[(P_x^2, P_y^2), (P_x, P_z)]$

Input cards:

```

4
4 0.25 -0.25 X 2 Y 2 X 1 7 1
4 0.25 -0.25 X 2 Y 2 7 1 X 1
4 0.25 -0.25 Y 2 X 2 X 1 7 1
4 0.25 -0.25 Y 2 X 2 7 1 X 1

```

Result:

***** THE TIME IS NOW = 4.268 SECONDS ***** CYCLIC:

```

      2 2 1 1      1 1 2 2
1/ 4 ( P P P P - F P P P )
      X Y X Z      7 X Y X
      2 2 1 1      1 1 2 2
1/ 4 ( F P P P - F P P P )
      X Y Z X      X 7 Y X
      2 2 1 1      1 1 2 2
1/ 4 ( F P P P - F P P P )
      Y X X Z      7 X X Y
      2 2 1 1      1 1 2 2
1/ 4 ( P P P P - F P P P )
      Y X Z X      X 7 X Y

```

EQUALS

```

      1
+IM *
      2 3      3 2
1 ( P P + P P )
      X Y      Y X
      4 1      1 4
-1 ( F P + F P )
      X Y      Y X
      2 1 2      2 1 2
1 ( P P P + P P P )
      X Y Z      7 Y X

```

```

      3
+IM *
      2 1      1 2
1 ( P P + P P )
      X Y      Y X
      3
1/ 2 P
      Y
      1 2      2 1
-1 ( P P + F P )
      Y Z      Z Y

```

B.2 REDUCTION OF SINGLE TERM

P P P P P P
x y x y z z

Input cards:

1
6 1.0 0.0 X 1 Y 1 X 1 Y 1 Z 1 Z 1

Result:

***** THE TIME IS NOW = 4.403 SECONDS ***** CYCLIC:

1 1 1 1 1 1
1 P P P P P P
X Y X Y 7 7

EQUALS

2 2 2
1 P P P
X Y Z

1
+IM *

1 1 1 3
1 P P P
X Y Z

2
+IM *

2 2
1 P P
X 7

B.3 COMMUTATOR ARISING FROM TRANSFORMATION TO MINIMAL SET

$$\left[\frac{1}{2} (P_x P_y P_z + P_z P_y P_x), \frac{1}{2} \{P_x^2, P_y^2\} \right]$$

Input Cards:

```

4
5 0.25 -0.25 X 1 Y 1 Z 1 X 2 Y 2
5 0.25 -0.25 X 1 Y 1 Z 1 Y 2 X 2
5 0.25 -0.25 Z 1 Y 1 X 1 X 2 Y 2
5 0.25 -0.25 Z 1 Y 1 X 1 Y 2 X 2
    
```

Result:

```

1 1 1 2 2 2 2 1 1 1
1/ 4 ( P P P P P - P P P P P )
      X Y Z X Y Y X Z Y X
1 1 1 2 2 2 2 1 1 1
1/ 4 ( P P P P P - P P P P P )
      X Y Z Y X X Y Z Y X
1 1 1 2 2 2 2 1 1 1
1/ 4 ( P P P P P - P P P P P )
      Z Y X X Y Y X X Y Z
1 1 1 2 2 2 2 1 1 1
1/ 4 ( P P P P P - P P P P P )
      Z Y X Y X X Y X Y Z
    
```

EQUALS

```

1
+IM *
2 4 4 2
-1 ( P P + P P )
   X Y Y X
4 2 2 4
1 ( P P + P P )
   X Y Y X
    
```

```

3
+IM *
4
2 P
   X
2 2 2 2
-5 ( P P + P P )
   X Z Z X
4
-2 P
   Y
2 2 2 2
5 ( P P + P P )
   Y Z Z Y
    
```

```

      5
+IM *
      2
-8  P
      X
      2
      8  P
      Y

```

B.4 DIPOLE MOMENT COMMUTATOR

$$[P_y^2, \Phi_x]$$

Input cards:

```

1
2  1.0 -1.0 Y 2  U 1

```

Result:

$$1 \begin{pmatrix} P_x P_y - P_y P_x \\ Y U & J Y \end{pmatrix}$$

EQUALS

```

      1
+IM *
      1 1      1 1
1 ( P P + P P )
      W Y      Y W

```

B.5 TRANSFORMING INTENSITIES

$$\left[\frac{1}{2} (P_x P_y P_z + P_z P_y P_x), \frac{1}{2} [P_x^2, \Phi_z] \right]$$

Input cards:

```

4
5  0.25 -0.25 X 1  Y 1  Z 1  X 2  W 1
5  0.25 -0.25 X 1  Y 1  Z 1  W 1  X 2
5  0.25 -0.25 Z 1  Y 1  X 1  X 2  W 1
5  0.25 -0.25 Z 1  Y 1  X 1  W 1  X 2

```

***** THE TIME IS NOW = 4.731 SECONDS *****

CYCLIC:

```

      1 1 1 ? 1      1 2 1 1 1
1/ 4 ( P P P P P - P P P P P )
      X Y Z X W      W X Z Y X
      1 1 1 1 2      ? 1 1 1 1
1/ 4 ( P P P P P - P P P P P )
      X Y Z W X      Y W Z Y X
      1 1 1 ? 1      1 2 1 1 1
1/ 4 ( F F F P P - P P P P P )
      Z Y X X W      W X X Y Z
      1 1 1 1 2      2 1 1 1 1
1/ 4 ( P P P P P - P P P P P )
      Z Y X W X      X W X Y Z
  
```

EQUALS

1
+IM *

```

      1 2 2      ? 2 1
-1 ( P P P + P P P )
      W X Y      Y X W
      1 2 2      ? 2 1
1 ( P P P + P P P )
      W X Z      Z X W
      1 3 1      1 ? 1
-1/ 2 ( P P P + P P P )
      U X Z      Z X U
      1 2 1 1      1 1 2 1
1/ 2 ( P P P P + P P P P )
      V X Y Z      Z Y X V
  
```

2
+IM *

```

      1 1 1      1 1 1
-3 ( P P P + P P P )
      U X Z      Z X U
      1 1 1      1 1 1
2 ( F P P + P P P )
      V Y Z      Z Y V
      1 2      ? 1
-3/ 2 ( P P + P P )
      W Y      Y W
      1 2      2 1
3/ 2 ( P P + P P )
      W Z      Z W
  
```

5
+IM *

```

      1
-1/ 2 P
      W
  
```

2 1 ?
+ P F P)
7 Y X

1 ?
P P)
Y X

2 1
P P)
Z Y