UTIL.MAN

In this manual we describe all the options concerning :

- THE MANIPULATION OF VECTORS .
- THE INTERACTION FILES .

They can be used in the 2 codes : ANTOINE OR NATHAN.

- **61.** **List all the vectors of files.**
- **62.** **Copy vectors.**
- **63.** **Change the precision of vectors.**
- **64.** **Overlap between vectors of a file.**
- **65.** **Overlap between vectors of 2 different files.**
- **66.** **Overlap between vectors of many files (one by one).**
- **67.** **Orthogonalization of a vector .**
- **68.** **Linear combination of vectors .**
- **69.** **Ordering of states with energy.**
- **70.** **Spectrum.**
- **71.** **Spectrum without ordering.**
- .....
- **81.** **Calculation of specific interactions**
- **82.** $0\nu\beta\beta$ **TBME.**
- **83.** **Center of Mass Hamiltonian.**
- **84.** **Center of Mass Hamiltonian for nocore.**
- **85.** **Information about interactions.**
- **86.** **Modifications of an interaction**

- **87.** **Addition of interactions**
- **88.** **Addition of NucL+Coulomb.**
- **89.** **Substitution of TBME**
- **90.** **Substitution of monopoles**
- **91.** **Density dependance with A**
- **92.** **Creation of a H file from standard TBME.**
- **93.** **Creation of H with random TBME.**
- **94.** **Rewrite H nocore for standard calculation.**
- **95.** **Creation of H files for fit .**

61. **List all the vectors of files.**

```
 61  0  0  0
  3 10 -11 12                  a)

a)   NFIL,(FILV(k),k=1,NFIL)
```

a) All the vectors of the files FILV are read and the characteristics are printed . Remember that if FILV is negative , the file is not rewinded.

62. **Copy vectors.**

```
 62  1  0  0
new text
 -20 10  0 0   0               a)

a)   (FILV(k),k=1,2),(INIV(k),k=1,2), NCAL
```

a) Like always : FILV(1) final file. FILV(2) initial file. INIV initialization of the files. NCAL number of vectors to copy. If NCAL=0 we go until the end of the file .

Notice that this option can be used to change the "TEXT" of vectors.

63. **Change the precision of vectors.**

```
 63  0  0  0
  11 10  0 0   0               a)

a)   (FILV(k),k=1,2),(INIV(k),k=1,2), NCAL   a)
```

a) Idem precedent option. Notice that it transforms double precision in simple (usual case) but do also the opposite .

64. Overlap between vectors of a file.

```
 64  0  0  0
  10 0 0

a)   FILV,INIV,NCAL   a)
```

a) Overlaps between the vectors of the file FILV are calculated only if the valence space, the dimensions ... are the same. In M scheme the time reversal symetry must be the same

65. Overlap between vectors of 2 different files.

```
 65  0  0  0
  11 10  0 0   0              a)

a)   (FILV(k),k=1,2),(INIV(k),k=1,2),(NCAL(k),k=1,2)   a)
```

a) standart reading. NCAL(k) number of vectors on each file. Same condition than the precedent option .For each state of FILV(1) we loop on all the vectors of FILV(2).

66. Overlap between vectors of many files (one by one).

```
 66  0  0  0
3  11 10 13 0 0 0 4            a)

a) NFIL,(FILV(k),k=1,NFIL),(INIV(k),k=1,NFIL),NCAL
```

a) we loop on NCAL , the corresponding vectors on each file FILV must have the same type (if not the code stops). Ovelap betwwen all the possible files are calculated . This option is especially used to compare vectors calculated with different interactions.

67. Orthogonalization of a vector .

```
 67  0  0  0
  11 10 13 0 0 0 4            a)

a) (FILV(k),k=1,3),(INIV(k),k=1,3),NCAL
```

a) we Take ONE state on FILV(2), we orthogonalize at NCAL states of FILV(3), the result (normalized) is written on FILV(1).

68. Linear combination of vectors .

```
 68  0  0  0
  11 10 0 0 2            a)
  1.0 1.0                B)

a) (FILV(k),k=1,2),(INIV(k),k=1,2),NCAL
b) (ZCF(k),k=1,NCAL)
```

a,b) we take the linear combination of the NCAL vectors of FILV(2) with the weight ZCF(k). Result is normalized and store on FILV(1).

69. Ordering of states with energy.

```
 69  0  0  0
  11 10 0 0 5            a)

a) (FILV(k),k=1,2),(INIV(k),k=1,2),NCAL
```

a) States of FILV(2) are ordered and written on FILV(1) .

70. Spectrum .

```
 70  0  0  0
2 11 10 0 0 5 4          a)

a) NFIL,(FILV(k),k=1,NFIL),(INIV(k),k=1,NFIL),(NCAL(k),k=1,NFIL)
```

Spectrum calculated with all the read states.

71. Spectrum without ordering.

```
 70  0  0  0
2 11 10 0 0 5 4          a)

a) NFIL,(FILV(k),k=1,NFIL),(INIV(k),k=1,NFIL),(NCAL(k),k=1,NFIL)
```

a) data idem precedetn option . The spectrum is not ordered . (it allows an easier comparison betwwen different spectra).

81. Calculation of specific interactions

```
81 1 0 0
Quadrupole-Quadrupole
   95   4    307 1103 305 1101                    a)
    1     0.1 0.2                                 b)

a)  FIL, SH, (NLJ( k ), k= 1, SH)
b)  ICAS, (XQ( k ), k= 1, 2)
```

a) SH= number of shells, NLJ(k)= nlj (like always)
Individual energies are put at 0.
b) Calculation is done in proton-neutron formalism (but written in isospin)
XQ(1)= coefficient for pp, XQ(2)= coefficient for pn.
Interactions ICAS =

1 : Quadrupole.
2 : Hexadecapole.
3 : Octupole.
4 : Orbital.
5 : Spin.
6 : Pairing T=1
7 : Pairing T=0

For pairing XQ(2) is not relevant.

82. $0\nu\beta\beta$ TBME.

```
82 0 0 0
0 80 48 -1 -1                       a)
4 307 1103 305 1101                 b)
7.72 950.  1  1                     c)

a)  DEL,FLMAT,MASSE,LQ,PI
b)  SH,(NLJ(K),K=1,SH)
c)  ZENER,ZLB,ISRC,IFNS
```

a) DEL=0 FLMAT= file for TBME LQ=PI=-1
b) valence space
c) ZENER (see in ybb0.f value following the nucleus) ZLB=950.
ISRC=1 short range correction =0 no ... IFNS=1 Finite size correction =0 no ...

83. Center of Mass Hamiltonian.

```
 83 1 0 0
HCM cor Ca40
99   6 15                                    a)
1 103 101 205 203 1001 307 305 1103 1101 409 407 1205 1203 2001  b)

a)           FLHCM,NCOR,SH
b)          (NLJ(k),k=1,SH)
```

FLHCM file of Hcm. The NCOR first shells of NLJ are in the core.
A standard H file is created .

84. Center of Mass Hamiltonian for nocore.

```
 84 0 0 0
  11 12                                      a)

a)    N1MAX, N2MAX
```

Creation of a center of mass file to be used in nocore calculations .
N1MAX= 2n+l of the last shell in the valence space.
N2MAX= (n1+n2) maxi of TBME.
11 12 t=10 for nuclei of the p shell.
6 8 t= 4 for nuclei of the sd shell.
20 20 t=20 for He4 ...

85. Information about interactions

```
 33  0 0
  2 90 91                                                a)
0 1 4 307 1103 305 1101  0.4                             b)

a)   NFIL, (FIL( k ), k= 1, NFIL)  \\
b)    TMINI,TMAXI,SH,(NLJ(i),I=1,SH), ZLIM
```

TMINI,TMAXI : isospin min et max.
We calculate "norm" and "overlap" of interactions:
N^2(q)=$\sum_{mnpq,jt}$ (2j+1)(2t+1)V(mnpq,jt,q)*V(mnpq,jt,q)/ $\sum_{mnpq,jt}$ (2j+1)(2t+1)
Summation is done on all the jt TBME allowed by the Pauli principle.
O(q1,q2)=$N^2(q1,q2)/(N(q1)$*N(q2))
We compare the monopoles. If a TBME differs more than ZLIM, it is printed .

86. Modifications of an interaction

```
 86 1 0 0
KB3 with modif
   99 90   1.0 1.0   0.0 0.0                          a)
      0.0  0.0  0.0  0.0                              b)
       307 307  0.2                                   c)
       307 305  0.1                                   c)
        0  307  0.2                                   c)
    0  -1  307  0.                                    d)
    0  307 307  0.1                                   d)
    1  307 307  0.1                                   d)
    0   0  307  0.2                                   d)

a)  (FIL( k ), k=1,2), ZPDIA, ZPNDIA
b)  (ZD( k ), k=1,SH)
c)  (PAIR( i ), i=1,2), VPAIR
d)  ISO , (MONO( i ), i=1,2), VMONO
```

a) FIL(1)= new H FIL(2)= old H
ZPDIA =global diagonal pairing added
ZPNDIA=global non-diagonal pairing added
b) modification of individual energies. Loop on TMAX

c) Modifications of matrix elements of pairing.
PAIR(i,k)= nlj , VPAIR : modification of this specific pairing.
Terms are read until PAIR(1,k) =0 (in our example we have 2 pairing modifications)
d) Modification of the monopole. Same principle as for the Pairing. (ISO (k) is the isospin).
It is possible to initiate ALL the monopoles at 0 in taking in the first modification (like in our example) MONO(1,1)=-1

87. Addition of interactions

```
 87  1 0  0
 Iokin.sdfp+10*cdm
  3 99 92 93                                        a)
7 205 1001 203 307 1103 305 1101                    b)
  1.0  10.0                                         c)

a) NINT, FLRES,(FIL( k ), k= 1, NINT)
b)  SH,(NLJ( k ), k= 1, SH)
c)    (ZCOEF( k ), k= 1, NINT)
```

a) FLRES= file of the final interaction
b) valence space
c) ZCOEF= multiplicative coefficient for each interaction

On each file the matrix elements can be written in different orders or even not defined. The individual energies are also added.

88. Addition of NucL+Coulomb.

```
  88  1 0  0
  kb3+coulomb
98 90 95                  a)
 4 307 1103 305 1101      b)

a)  FLRES, FLNUC, FLCOUL
b)  SH,(NLJ( k ), k= 1, SH)
```

89. Substitution of TBME

```
89 0 0 0
1 99 93                   a)
 3     1103 305 1101      b)

89 1 0 0
KB3.FF-FR+GXPF.RR
2 98 90 99                a)
 4 307 1103 305 1101      b)

a) NINT, FLRES,(FIL( k ), k= 1, NINT)
b)   SH,(NLJ( k ), k= 1, SH)
```

a,b) idem option to add interactions .

Individual energies are those of the FIL(1).

Starting from the TBME defined in FIL(1), TBME defined in each new interaction replaced the matrix elements defined before.

In the present example rr TBME of GXPF1 (file 93) are extracted and in the second step are put in KB3 (file 90)

90. Substitution of monopoles

```
  90  1 0  0
 Iokin.sdfp with kb3 mono
   2 99 92 93                                    a)

a) NINT, FLRES, (FIL( k ), k= 1, NINT)
```

The valence space (with individual energies) is defined in FIL(1). If a monopole is defined in FIL(2), ..., FIL(NINT), it replaces the monopole of FIL(1).

91. Density dependance with A

```
  91 1 0 0
Iokin.sdfp for S44
   99 90 44 40  0.33333   a)

 FLWRI,FLLEC,AFIN,AINI,ZPO
```

multiplicative coefficient of all the TBME :
XMULT=(DBLE(AINI)/DBLE(AFIN))**ZPO

The new interaction is defined without density dependance . (This can be changed by hand).

92. Creation of a H file from standard TBME.

```
  92  1  0  0
 Bonn A for Tin region
   95  5  1 1205 407 1203 2001 511                  a)
     0.0 0.2  2.4 2.5 3.0                           b)
     1 50 50 0.3333333   0.0                        c)
       1 1 1 1    0 1      0.5                     d)
       .........
       5 5 5 5   11 0      0.2
       0 1 1 1    0 1      0.5

 a)          FLMAT,IMAT,SH,(NLJ(k),k=1,SH)
 b)         ((ZEPSI(k,t),k=1,SH),t=1,min(IMAT,2))
 c)           IDENS,P0,N0,ZDE,ZISO
 d)          I1,I2,I3,I4,J,T,(XX(k),k=1,N(T))
```

Rewriting the 2-body matrix elements in the format used in the shell model codes.

IMAT=1 V(T=1,pn)=V(nn)=V(pp) N(1)=1
IMAT=2 V(T=1,pn)=V(nn)≠V(pp) N(1)=2 nn,pp
IMAT=3 V(T=1,pn)≠V(nn)≠V(pp) N(1)=3 pn,nn,pp

i1,i2,i3,i4=numero of the shells $(a^+(i1)a^+(i2))^{jt}$ $(a(i3)a(i4))^{jt}$

This loop continues until the end or until we find i1=0 .

The code notes all the i1, i2, i3, i4 which appears and at the end prints only these matrix elements.

Check that i1 in the list is nlj(i1) ...

Some lists are written with T,J or 2J,2T or .... instead of J,T . It is easy to change the reading in the code (see zforma.f).

93. Creation of H with random TBME.

```
  93  0  0  0
```

```
  99 90 -1.0 1.0  1357                                  a)

a)   FLWRI,FLLEC,ZMIN,ZMAX,INIT
b)   ((Z(K,T),K=1,NC),T=1,TMAX)
```

a) FLLEC= file of the interaction which defines the valence space.
The new file (FLWRI)) will be identical at FLLEC with individual energies read (b) and TBME uniformed random between ZMIN and ZMAX . INIT is the integer which initiates the random numbers.

94. Rewrite H nocore for standard calculation.

```
 94  0  0  0
  99 95                                                a)
  5 6 8 10.

a)   FLWRI,FLLEC
b)    N1MAX,N2MAX,NPAR,ZHCM
```

a) FLLEC=file of the nocore H . (The text will be copied in FLWRI)

b) N1MAX,N2MAX see definition in option 84 (center of mass for nocore). NPAR= number of particles . ZCDM= coef for center of mass

95. Creation of H files for fit .

```
  95 0 0 0
  0                                          a)
2 3  205 1001 203                            b)
1 8 8 0.30 0.00                              c)
```

a) NINT,(FIL(K),K=1,NINT) b) ICAS,SH,(NLJ(K),K=1,SH) b) (IDENS(k),k=1,3), (Z(k),k=1,2)

To fit an interaction we create H files :
a) The NINT first are specific Hamiltonian (Q-Q , ...). The starting H will be definedelsewhere.

b) After these NINT H files we define K files corresponding at all the possible individual energies and TBME. These H are classified in different "groups" following the value of ICAS.
ICAS=1 epsilons, V(i,j,k,l,J,T)
ICAS=2 epsilons, M(i,j,T), W(i,j,k,l,J,T)
ICAS=3 Invariant transformation (A.Zuker):V(i,j,T), W(i,j,k,l,J,T)

V are the TBME, W are the TBME with monopole M substracted.

c) Density dependance (see comments on interaction files) . this density dependance must be identical at that of the NINT interactions and at that of the starting H .