BIGSTICK Density Matrix Format Specification

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This document specifies the format of the one-body density matrix files produced by the many-body code BIGSTICK.

```
  State       E         Ex          J        T
    1    -330.17116   0.00000      1.500   11.500
  Single particle state quantum numbers
ORBIT       N      L    2 x J
     1      0      2      3
     2      0      2      5
     3      1      0      1
 Initial state #     1 E = -330.17117 2xJ, 2xT =     3   23
 Final state   #     1 E = -330.17117 2xJ, 2xT =     3   23
 Jt =   0, proton       neutron
    1     1   1.55844    5.40558
```

0.1 Definition.

One-body density matrices between many-body eigenstates $|\Psi\rangle$ are defined as

$$\rho_K^{fi}(ab) = \frac{1}{\sqrt{2K+1}} \langle \Psi_f || [\hat{c}_a^\dagger \otimes \tilde{c}_b]_K || \Psi_i \rangle, \tag{1}$$

where $\hat{c}_a^\dagger$ is the fermion-creation operator (with good angular momentum quantum numbers), $\tilde{c}_b$ is the time-reversed fermion-destruction operator. The creation/destruction operators refer to single-particle states in a harmonic oscillator basis.

Each state $|\Psi_i\rangle$ and has an energy eigenvalue and two quantum numbers: total angular momentum J_i and total isospin T_i. The angular momentum K of the density matrix operator $\rho_K(ab)$ must satisfy conservation of angular momentum according to the triangle inequality rule for both the many-body states and the single-particle states:

$$|J_f - J_i| \leq K \leq |J_f + J_i|, \tag{2}$$

$$|j_a - j_b| \leq K \leq |j_a + j_b|. \tag{3}$$

0.2 Symmetry.

Two space saving measures may be taken in the storage of these matrix elements which must be taken into account. The first is trivial: matrix elements equal to zero are not stored in the file. The second is more subtle and can be confused with the first measure. One-body density matrices obey the following symmetry relation:

$$\rho_{K,T}^{i,f}(ba) = (-1)^{j_a - j_b + J_i - J_f + T_i - T_f} \rho_{K,T}^{f,i}(ab), \tag{4}$$

only matrix elements with $a < b$ (or $a > b$) need to be stored in order fully specify the nonzero matrix elements.

0.3 Filename.

The density matrix file ends in ".dres".

0.4 Format.

The file is written with standard plain text.

0.5 Three blocks.

The density matrix file has three consecutive blocks: (1) many-body state information, (2) single-particle state quantum numbers, (3) density matrix element blocks.

0.6 First block: States

The f and i indices on the $\rho_J^{f,i}(ab)$ object refer to the many-body states involved.

The states section of the file is identified by the following line:

```
  State       E          Ex          J        T
```

This line begins with exactly two blank spaces. Each state is specified by 5 numbers:
1. State number (i.e, 1, 2, 3, 4. 1 is the ground state.)
2. State eigenvalue/energy in MeV
3. State excitation energy (eigenvalue/energy minus the ground state (1st state) eigenvalue/energy)
4. State total angular momentum quantum number
5. State total isospin quantum number

Each number should be in its own column separated by one or more spaces.

Example with five states:

```
  State       E          Ex          J        T
    1    -330.17116    0.00000      1.500   11.500
    2    -330.13419    0.03697      0.500   11.500
    3    -329.77492    0.39624      2.500   11.500
    4    -329.70014    0.47102      1.500   11.500
    5    -329.42771    0.74346      3.500   11.500
```

0.7 Second block: Single particle state quantum numbers

The single particle state quantum numbers section begins with the following two lines:

```
  Single particle state quantum numbers
ORBIT       N      L    2 x J
```

Each single particle state (SPS) is specified by 4 numbers:
1. SPS number (i.e. 1, 2, 3, ...)
2. SPS nodal quantum number
3. SPS orbital angular momentum
4. SPS twice the total angular momentum

Each number should be in its own column separated by one or more spaces.

Example with five SPS:

```
  Single particle state quantum numbers
ORBIT       N      L    2 x J
     1      0      4      7
     2      1      2      5
     3      1      2      3
     4      2      0      1
     5      0      5     11
```

0.8 Third block: Density matrix element blocks

Density matrix blocks have three nested sub-blocks:
1. States involved
2. Transition angular momentum value
3. SPS labels and matrix elements

0.8.1 States involved

The states involved in a block are specified by two lines. The first specifies the initial (ket) state and the second specifies the final (bra) state.

By example:

```
 Initial state #    1 E = -330.17117 2xJ, 2xT =    3  23
 Final state   #    1 E = -330.17117 2xJ, 2xT =    3  23
```

Both lines are preceded by a space. "Initial" and "Final" are capitalized.

0.8.2 Transition angular momentum (operator momentum)

The operator connecting a given initial and final states is constrained by conservation of angular momentum, but can otherwise take any integer value. The line specifying this sub-block is as follows:

```
 Jt =   1, proton      neutron
```

The line begins with one space. The two strings at the end of the line indicate the coupling of the second two columns of density matrix elements that follow. For isospin format density matrix files, this line would be:

```
 Jt =   1, Tt = 0        1
```

0.8.3 Single particle state labels and matrix elements

The inner-most block of data store the actual one-body density matrix elements for each allowed combination of single-particle states. There are four numbers per line in the inner-most block:

1. Creation SPS label (a)
2. Destruction SPS label (b)
3. Proton (isospin-0) coupling one-body density matrix element $\rho^{f,i}_{K,(p)}(a,b)$ (if isospin format then $\rho^{f,i}_{K,T=0}(a,b)$)
4. Neutron (isospin-1) coupling one-body density matrix element $\rho^{f,i}_{K,(n)}(a,b)$ (if isospin format then $\rho^{f,i}_{K,T=1}(a,b)$)

For example:

```
    1    1   1.55844   5.40558
    2    2   0.82990   4.64991
    3    3   0.33371   2.66182
    4    4   0.15089   2.19140
    5    5   0.19585   5.45541
```

Matrix elements which are identically zero are not stored in the file to save space.

0.9 Example density matrix file with one state

From the following example file one should be able to find that (examples):

$$\rho^{f=1,i=1}_{K=0,(p)}(a=3,b=3)=0.33371 \tag{5}$$

$$\rho^{f=1,i=1}_{K=2,(n)}(a=2,b=1)=-0.00432 \tag{6}$$

```
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```

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    1    1   1.55844   5.40558
    2    2   0.82990   4.64991
    3    3   0.33371   2.66182
    4    4   0.15089   2.19140
    5    5   0.19585   5.45541
 Jt =   1, proton       neutron
    1    1   0.01905   0.02637
    1    2  -0.00378   0.01404
    2    1   0.00378  -0.01404
    2    2   0.01022   0.00476
    2    3   0.00387   0.00942
    3    2  -0.00387  -0.00942
    3    3  -0.00075   0.82318
    3    4   0.00046   0.01952
    4    3  -0.00046  -0.01952
    4    4  -0.00194  -0.01399
    5    5   0.00030   0.00399
 Jt =   2, proton       neutron
    1    1  -0.13193   0.00294
    1    2   0.04339   0.00432
    1    3  -0.08074  -0.00145
    2    1  -0.04339  -0.00432
    2    2  -0.08825   0.00628
    2    3  -0.03159   0.00310
    2    4  -0.04636   0.01764
    3    1  -0.08074  -0.00145
    3    2   0.03159  -0.00310
    3    3  -0.02227  -0.36934
    3    4   0.02059   0.01636
    4    2  -0.04636   0.01764
    4    3  -0.02059  -0.01636
    5    5  -0.01075  -0.21205
 Jt =   3, proton       neutron
    1    1   0.00550   0.01229
    1    2   0.00022   0.01318
    1    3  -0.00009   0.01506
    1    4  -0.00175  -0.01271
    2    1  -0.00022  -0.01318
    2    2   0.00253  -0.01080
    2    3   0.00111  -0.00630
    2    4   0.00051   0.00261
    3    1  -0.00009   0.01506
    3    2  -0.00111   0.00630
    3    3   0.00033   0.82699
    4    1   0.00175   0.01271
    4    2   0.00051   0.00261
    5    5   0.00029   0.00712
```