

The contents in grey are just to explain the formats expected by the code. They **must** be deleted before you use the example below.

"PandasCommute/input/pn.sp"

! usdb.sp comment lines headed with "!", you can add as many such lines as possible, as long as they are all headed with "!"

pn pn scheme, used in NushellX, necessary after comment lines

16 8 A Z of the core, necessary after "pn" the upper line

6 total number of neutron and proton orbits, expected after the upper line

2 3 3 2 types of particles, 3 proton orbits and 3 neutron orbits, necessary

1 1 2 3 info of proton orbits, N=1, l=2, j=3/2 (0d5/2).

2 1 2 5 the sequence number does not matter in PandasCommute, but the N, l, j values are very important.

3 2 0 1

1 1 2 3 1st neutron orbit, 0d3/2

2 1 2 5

3 2 0 1

"PandasCommute/input/GMEpn.int"

! orbits 1-3 protons, 4-6 neutrons comment lines headed with "!", to be skipped. Again, there can be as many comment lines as you want, as long as they are headed with "!"

!SP ORB N L J Tz

!SP 1 0 2 3/2 1

!SP 2 0 2 5/2 1

!SP 3 1 0 1/2 1

!SP 4 0 2 3/2 -1

!SP 5 0 2 5/2 -1

!SP 6 1 0 1/2 -1

158 2.111700 -3.925700 -3.207900 2.111700 -3.925700 -3.207900

158 two-body matrix elements and 6 s.p.e.s in the sd shell. These are important, if 158 the number is not correct, dynamic memory can be not enough and the code breaks down. The 6 s.p.e. energies are also expected as float numbers, separated with blank spaces in a line.

2 2 2 2 0 1 -2.559800 a b c d J T V(abcd;JT)

2 2 1 1 0 1 -3.102500

2 2 3 3 0 1 -1.560200

1 1 1 1 0 1 -1.899200

1 1 3 3 0 1 -1.015000

3 3 3 3 0 1 -1.691300

2 1 2 1 1 1 0.655600

2 1 1 3 1 1 -0.045600

1	3	1	3	1	1	0.515800
2	2	2	2	2	1	-1.000700
2	2	2	1	2	1	-0.213700
2	2	2	3	2	1	-0.931700
2	2	1	1	2	1	-1.218700
2	2	1	3	2	1	0.886600
.....						

"PandasCommute/input/F.coef"

! orbits 1-3 protons, 4-6 neutrons Comment lines headed with "!"

!SP ORB N L J Tz

!SP 1 0 2 3/2 1

!SP 2 0 2 5/2 1

!SP 3 1 0 1/2 1

!SP 4 0 2 3/2 -1

!SP 5 0 2 5/2 -1

!SP 6 1 0 1/2 -1

K= 1 pF= 1 Angular momentum K and parity pF of the transition operator.

The code just picks up the first 2 integers out of whatever else in this line, and crown them K and pF in the code. This line is expected right after comment lines.

1 4 1.549193 a b Fab

1 5 -3.098387

2 4 3.098387

2 5 -2.898275

3 6 -2.449490

4 1 1.549193

4 2 -3.098387

5 1 3.098387

5 2 -2.898275

6 3 -2.449490