NuShellX Tutorial

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Outline

- How to obtain NuShellX.
- Starting NushellX
- Calculating Spectra
- Calculating transitions.

How to Obtain NuShellX

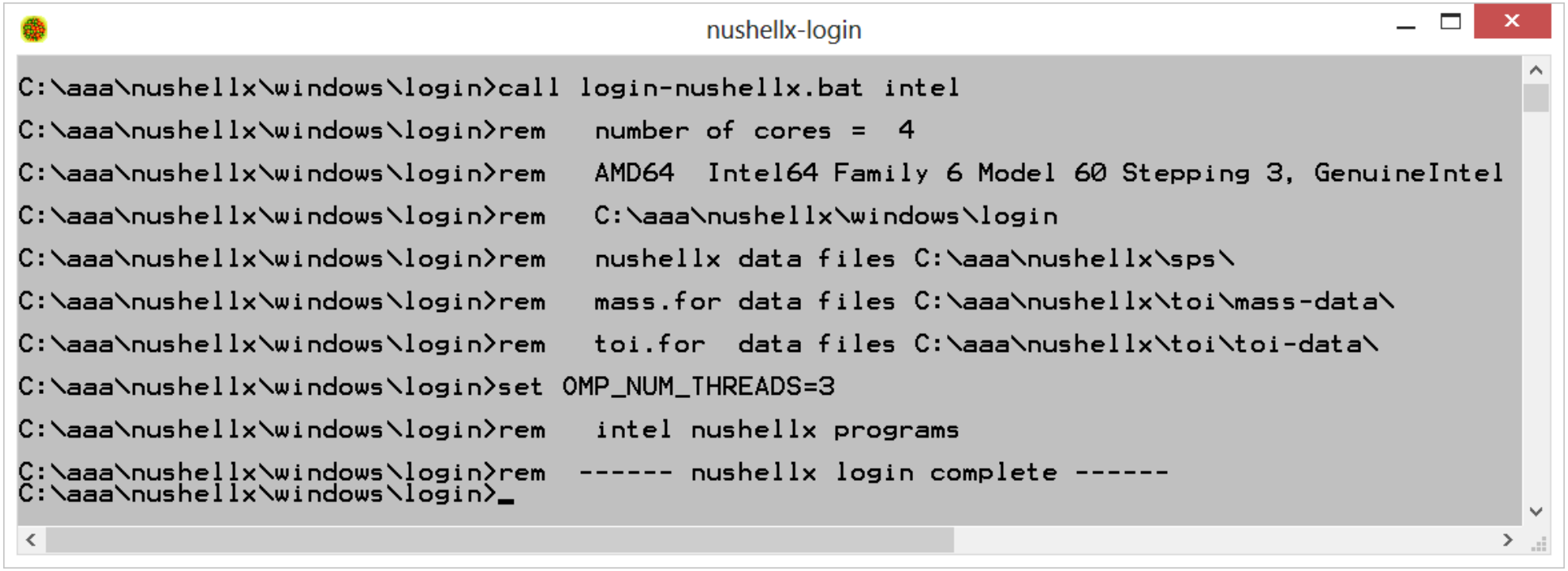
- From B. A. Brown's website
  - NuShellX@MSU for Windows PC can be obtained by sending an email to:
    - » brown@nscl.msu.edu
  - This version runs directly on any Windows PC without the need for any other software.
  - NuShellX@MSU is an adaption of W.D.M.Rae's code NuShellX with input and output files similar to the older Oxbash code.
  - W.D.M Rae's original version of the code can be obtained at his website.
    - » http://www.garsington.eclipse.co.uk/
- There are versions of NuShellX that are made to run on different platforms.
  - As far as I know only the windows version is kept up to date so be aware that the versions for different platforms may be inconsistent.

Starting NuShellX -login

- NuShellX is designed to be used with a special terminal window.
  - The window has commands aliased in a way that is supposed be independent of the platform used.
  - This is important because NuShellX is designed to set up and run the shell model interactions using scripts to run different programs and manage their inputs and outputs.
- To start this terminal window find the shortcut in the login directory:
  - The windows example is:
    - » C:\aaa\nushellx\windows\login
    - » “nushellx-login” is the name of the shortcut
    - » You can relocate this shortcut wherever is convenient for you.
- The “nushellx-login” shortcut runs the “login-nushellx.bat” script this script sets up the terminal used for nushellx calculations.
  - You may need to modify this file to suit your purposes.
  - It is recommended that you change the “OMP_NUM-THREADS” variable to 1 less than the number of cores on your machine so that you reduce contention with your operating system.

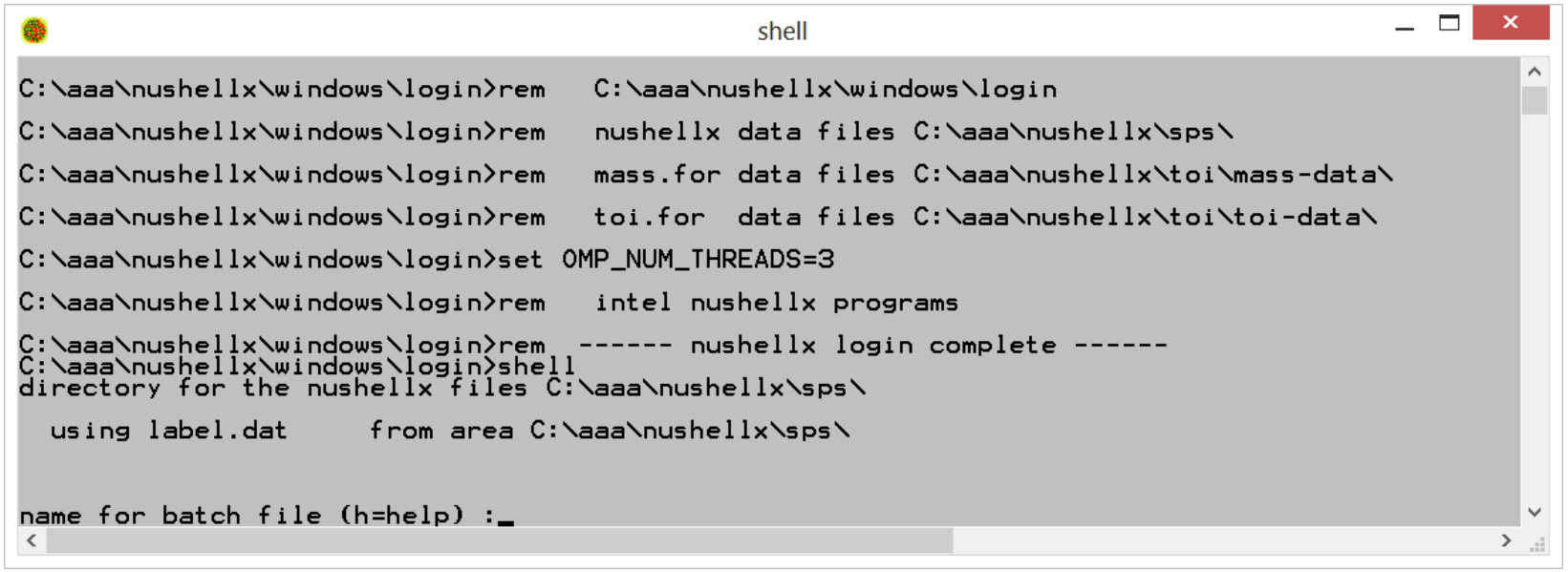
Example NuShellX -login

- Below is an example of the nushellx terminal window.
  - The login script is set up to print information about the system on startup.
- Take a moment and start your own terminal window.
  - Verify the OMP_NUM_THREADS is a reasonable value for your system.



Calculation of ^{20}Ne Spectrum

- The simplest operation in NuShellX is to calculate the spectrum of a single nucleus.
- The first step is to specify the parameters of the calculation and generate the script that will run the calculation.
  - This is done by running the program “shell” in the terminal window.
  - Be sure to navigate to an empty directory because many files will be created.
  - Simply type shell and press enter.



Calculation of ^{20}Ne Spectrum

- Enter a name for the batch file.
  - It is useful to have a naming convention that distinguishes what type of calculation is done.
    - » Here we will name it after the nucleus we intend to calculate: “ne20”.
- We want option “lpe”
  - “lpe” is the option to calculate wave functions and spectra.
    - » The ”lpe” option will be used before any other calculation.
  - The “den” option is for calculating wave function overlaps.
    - » We will discuss this in later slides
  - “help” will provide more information.
  - “st” ends the generation of the batch file.
    - » You can put as many calculations in the batch file as you wish.

Calculation of ^{20}Ne Spectrum

- Next you will be prompted for the model space name: input “sd”.
  - The model space names can be found in the first column of the file “label.dat” in the directory following directory
    - » C:\aaa\nushellx\sps
    - » This file is an input to NuShellX and the file path is always printed when shell is run.
  - The model space refers to the single particle orbitals that the valence particles can occupy.
    - » “sd” refers to the 1s0d shell of the harmonic oscillator.
    - » It is critical to choose the appropriate model space for your problem.
- You will be asked if you wish to restrict the model space. Press enter.
  - A blank answer is the same as “n” for no.
  - You may wish to do this if you are calculating in a large space.
  - It is not recommended to limit your model space unless absolutely necessary.

“label.dat”

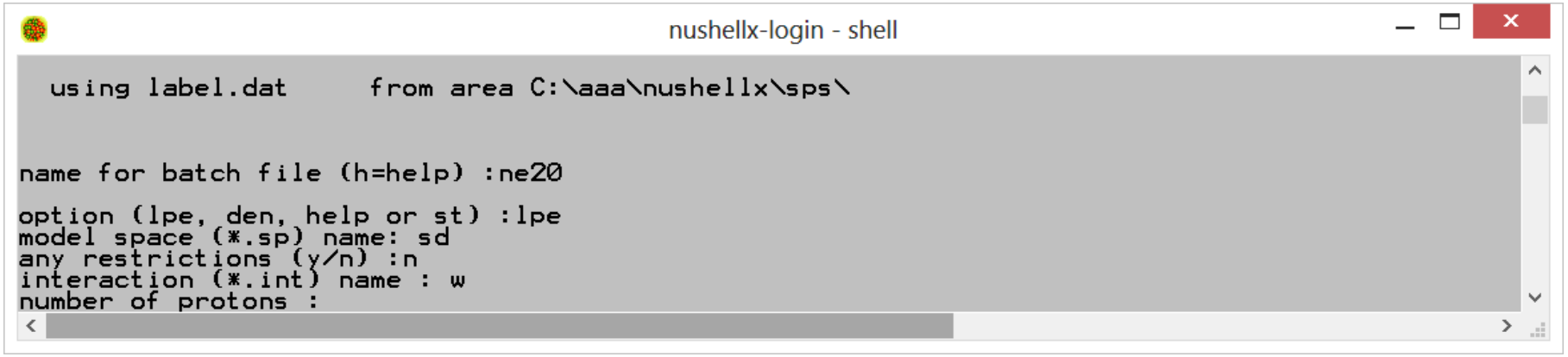
- Model space (*.sp file) name (single-particle state file name)
- Interaction (*.int file) name
  - In some cases the interaction may consist of several pieces which are read into MATRIX separately. In this case this interaction name is the code word which tells SHELL which *.INT files to include.)
- Model space code used for the output files
  - (The labels "p" and "n" should be reserved for charge-dependent interaction names)
- Interaction code used for the output files
- References and information

```
!   Reference list for model spaces (* is reserved)
!   (3) (1)             (3) (1)         (3) (1)       (3) (1)
!    a   p,ppn           h   ho,f5p      o             v   jj56pn,jj67pn,PBPOP
!    b   sd,sdpn,sdw     i   gl,jj45     p   *         w   pb206
!    c   zbm,zbmpn,zbme  j   slg         q   jj55pn    x   *
!    d   psd,psdpn       k   sns         r   jj45pn    y
!    e   f7,f7pn         l   sdpf,sdpfpn s             z
!    f   fp,fppn         m   n82         t   SPSDPF
!    g   d3f7,d3f7pn     n   *           u   i13
!    list of available model-space and interaction combinations
                         ! ---------------------------------------------
!(1)    (2)    (3) (4)   (5)
                         ! ---------------------------------------------
                         ! P Model Space
                         ! 1p1/2,1p3/2 orbits
p       ckpot    a   a   ! (8-16)POT    S. Cohen and D. Kurath,
p       cki      a   b   ! (6-16)TBME   Nucl. Phys. A73, 1 (1965) and
p       ckii     a   c   ! (8-16)TBME   Nucl. Phys. A101, 1 (1967)

p       pmom     a   d   ! Includes fit to moments, van Hees et al,
                         ! Nucl. Phys. A476, 61 (1988) and pri. comm.
p       pjp      a   e   ! JULIES-RICHTER POT INT
p       pjt      a   f   ! JULIES-RICHTER TBME INT
                         ! S. Afr. Tydskr.Fis. 15 nr. 3/4 (1992)
p       mp       a   g   ! D.J.MILLENER (PRIVATE COMMUNICATION NOV 1984)
p       pewt     a   h   ! * P(10-16)T: WARBURTON A=10-16 TBME INT (1991)
p       pwt      a   i   ! * P(5-16)T:  WARBURTON A= 5-16 TBME INT (1991)
p       pkuo     a   j   ! * Kuo, Paris interaction, Private Comm. (1989)
p       psu3     a   k   ! * SU3 INT - OCT 1990 VERSION
p       ckihe    a   l   ! * CKI plus fit to He isotopes PRC37, 2220 (1988).
```

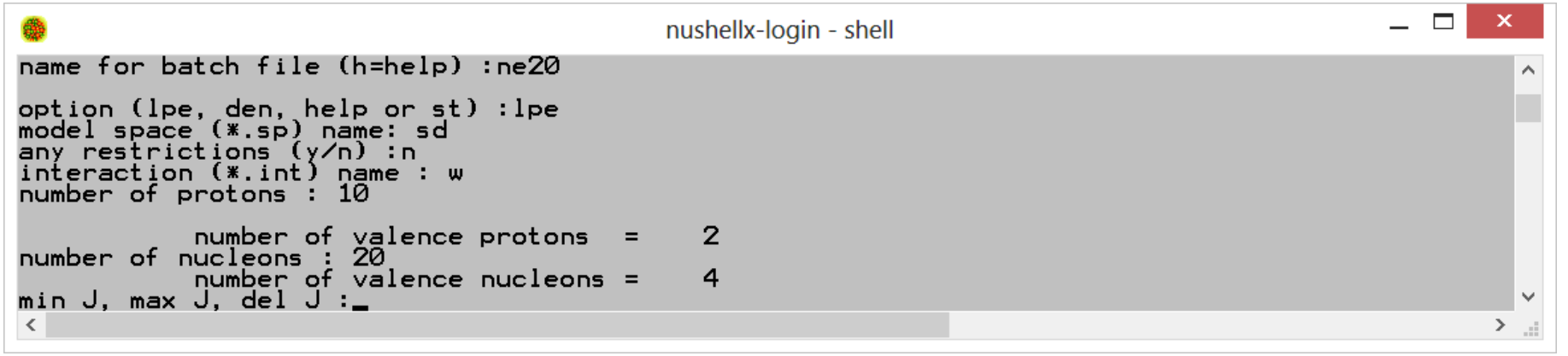
Calculation of ^{20}Ne Spectrum

- The interaction we will use is “w”:
  - The interaction name can be found in the second column “label.dat” file.
  - The selection of the appropriate interaction is critical to the validity of a calculation.
    - » Warning! Not all interactions in the sps directory are intended for the end user.
  - The “label.dat” has literature references for some interactions listed in the rightmost column.
    - » An example row of “label.dat”
      - sd w b w ! (W) WILDENTHAL'S A=17-39 "USD" INT (JULY 1982)
    - » It is recommended that you check the literature for the interaction you use before drawing any conclusions from the results of your calculation.



Calculation of ^{20}Ne Spectrum

- You will be prompted to enter the number of protons: “10”
- Number of nucleons is “20”
  - The terminal will display the number valence protons and the number of valence nucleons.
    - » It is a good idea that you check to see if your idea of the many body problem matches up with the output.
    - » If this doesn’t seem right make sure your model space, proton, and nucleon numbers are correct.
    - » Hint: negative numbers are bad.

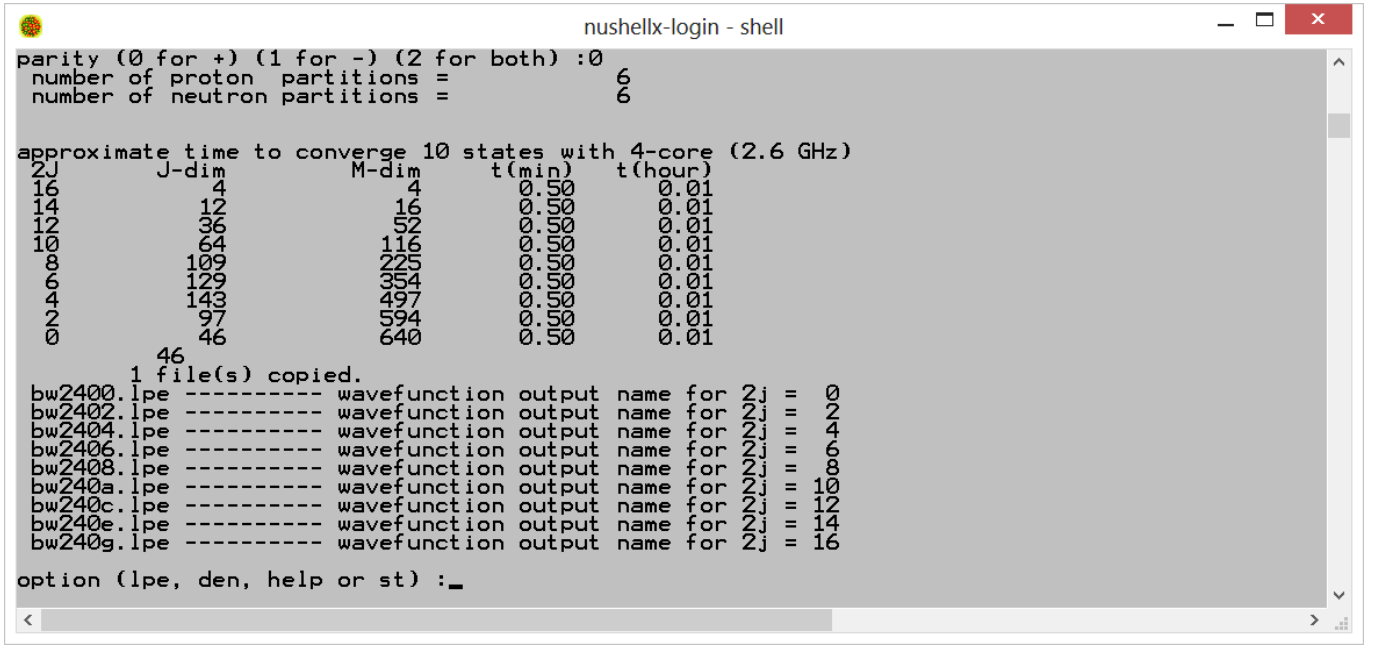


Calculation of ^{20}Ne Spectrum

- Min J, max J, del J: “0.0, 8.”
  - Omitting the “del J” argument is equivalent to using “1.0”
  - It is recommended that you calculate all values of angular momenta that you desire at the same time to take advantage of your processor’s parallelism.
    - » Don’t make different batch files for individual angular momentum values.
  - Restricting the momentum is one way to reduce the runtime of the calculation.
- Parity “0”
  - Restricting parity is another way to reduce the runtime of calculations.
- Shell will output an estimate of the runtime for the different angular momentum partitions.
  - Check this before you run a calculation for the first time so you know what to expect.
  - If any runtime is very large think about what types of restrictions you can make to the angular momentum and parity.
    - » It is also possible to restrict the number of eigenvalues calculated for each partition
    - » Only as a last resort should you restrict your model space.

Calculation of ^{20}Ne Spectrum

- After the runtime estimates for the different partitions shell will output the wavefunction output names.
  - These will be important for calculating transitions which we will discuss later.
- You will be prompted to enter another option: “st”
  - This tells shell you are done specifying a calculation and it should write the batch file.
  - If you enter lpe or den you can specify more calculations to be added to the batch file.



The ".ans" file

- This file stores the answers to shell so the batch file can be produced on demand.
- This is useful for producing large numbers of batch files using your own code or reproducing a calculation from someone else.
- It is also useful if you are prone to typos.
- To use the ".ans" file generated in our example type the command:
  - "shell ne20.ans"
  - The contents of this file are shown below.

```
------------------------------------------------
lpe,   0              ! option (lpe or lan), neig (zero=10)
sd                    ! model space (*.sp) name (a8)
n                     ! any restrictions (y/n)
w                     ! interaction (*.int) name (a8)
 10                   ! number of protons
 20                   ! number of nucleons
 0.0, 8.0, 1.0,       ! min J, max J, del J
  0                   ! parity (0 for +) (1 for -) (2 for both)
------------------------------------------------
st                    ! option
```

Calculation of ^{20}Ne Spectrum

- You have exited shell and now will be prompted to run the batch file.
  - This will execute a series of programs to generate the outputs that we specified.
- Simply type the name you entered at the first prompt:"ne20"
  - It should take less than a minute.
  - Many hundreds of output files will be generated.
    - » I have no idea what the function is of most of these files.
- NuShellX always generates some human readable output summaries that contain useful information.
  - For the spectrum of the nucleus look for an ".lpt" file that starts witht the batch file name.
    - » In our example it is: "ne20w.lpt"

```
------------------------------------------------------------
a =  20 z = 10
w                1.00000      0.96889  1.6466 -3.9478 -3.1635
```

N	NJ	E(MeV)	Ex(MeV)	J	T_z	p	lowest Ex	name
1	1	-40.491	0.000	0	0	1	0.000	bw2400.lpe
2	1	-38.715	1.776	2	0	1	1.776	bw2404.lpe
3	1	-36.278	4.212	4	0	1	4.212	bw2408.lpe
4	2	-33.735	6.756	0	0	1		bw2400.lpe
5	2	-33.175	7.316	2	0	1		bw2404.lpe
6	1	-31.976	8.515	6	0	1	8.515	bw240c.lpe
7	2	-30.517	9.974	4	0	1		bw2408.lpe
8	3	-30.343	10.148	2	0	1		bw2404.lpe
9	1	-30.261	10.230	3	0	1	10.230	bw2406.lpe
10	4	-30.054	10.437	2	0	1		bw2404.lpe
11	3	-29.815	10.676	4	0	1		bw2408.lpe
12	5	-29.754	10.736	2	0	1		bw2404.lpe
13	2	-29.745	10.746	3	0	1		bw2406.lpe
14	4	-29.604	10.886	4	0	1		bw2408.lpe
15	1	-29.295	11.196	1	0	1	11.196	bw2402.lpe
16	3	-29.054	11.436	3	0	1		bw2406.lpe
17	1	-28.903	11.588	5	0	1	11.588	bw240a.lpe
18	1	-28.900	11.591	8	0	1	11.591	bw240g.lpe
19	5	-28.738	11.752	4	0	1		bw2408.lpe

Calculation of ^{20}Ne Spectrum

- The states are indexed in the first column in order of energy.
- The J_π partition is indexed in the second column.
  - The first three states are the first state of their partition.
  - The 4th state is the second 0_+.
- The third column is the absolute energy of the eigenstate.
- The fourth column is the energy relative to the lowest energy state calculated.
  - This is not necessarily the ground state.

```
------------------------------------------------------------
a =  20 z = 10
w              1.00000      0.96889  1.6466 -3.9478 -3.1635
```

N	NJ	E(MeV)	Ex(MeV)	J	T_z	p	lowest Ex	name
1	1	-40.491	0.000	0	0	1	0.000	bw2400.lpe
2	1	-38.715	1.776	2	0	1	1.776	bw2404.lpe
3	1	-36.278	4.212	4	0	1	4.212	bw2408.lpe
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5	2	-33.175	7.316	2	0	1		bw2404.lpe
6	1	-31.976	8.515	6	0	1	8.515	bw240c.lpe
7	2	-30.517	9.974	4	0	1		bw2408.lpe
8	3	-30.343	10.148	2	0	1		bw2404.lpe
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18	1	-28.900	11.591	8	0	1	11.591	bw240g.lpe
19	5	-28.738	11.752	4	0	1		bw2408.lpe

Calculation of ^{20}Ne Spectrum

- The fifth column is the angular momentum.
- The sixth column is the isospin projection.
- The seventh column is the parity.
  - In our example the parity is always 1 (for plus) because we restricted the parity we calculated.
- The eighth column has the energy relative to the least energy state only if it is the first state of a given J_π.
- The ninthth column names the output file of the wave functions.
  - These are useful for calculations of wave function overlap.

```
------------------------------------------------------------
a =  20 z = 10
w              1.00000      0.96889  1.6466 -3.9478 -3.1635
```

N	NJ	E(MeV)	Ex(MeV)	J	T_z	p	lowest Ex	name
1	1	-40.491	0.000	0	0	1	0.000	bw2400.lpe
2	1	-38.715	1.776	2	0	1	1.776	bw2404.lpe
3	1	-36.278	4.212	4	0	1	4.212	bw2408.lpe
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17	1	-28.903	11.588	5	0	1	11.588	bw240a.lpe
18	1	-28.900	11.591	8	0	1	11.591	bw240g.lpe
19	5	-28.738	11.752	4	0	1		bw2408.lpe

Wave function file names

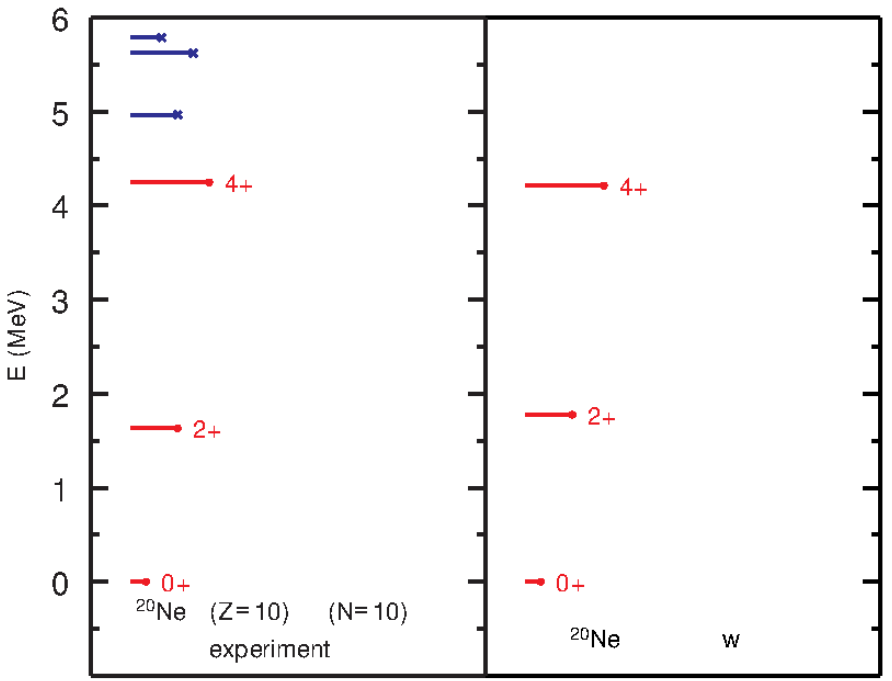
- The name of the wave function files contains information about the states they describe.
- Example: bw240c.lpe
  - "b" is the symbol for the model space found in label.dat
    - » Here b stands for the "sd"
  - "w" is the symbol for the interaction found in label.dat
    - » "w" happens to be the name of the potential as well bu this is not always the case.
  - "2" symbol for the number of valence protons
    - » Happens to be the number of valence protons but this is true only of single digit numbers.
    - » See the table to the right
  - "4" is the symbol for the number of valence nucleons.
  - "0" is the symbol for the parity
    - » 0 for + and 1 for -
  - "c" is the symbol for two times the spin.
    - » 12 in this case
    - » This means the spin is 6.
- The table to the right comes from the help file
    - » C:\aaa\nushellx\help

The symbols for J, T and N correspond to the following numbers

0 - 0	k - 20	f - 40	0 - 60	h - 80	f - 100	0 - 120
1 - 1	l - 21	g - 41	1 - 61	l - 81	g - 101	1 - 121
2 - 2	m - 22	h - 42	2 - 62	m - 82	h - 102	2 - 122
3 - 3	n - 23	i - 43	3 - 63	n - 83	i - 103	3 - 123
4 - 4	o - 24	j - 44	4 - 64	o - 84	j - 104	4 - 124
5 - 5	p - 25	k - 45	5 - 65	p - 85	k - 105	5 - 125
6 - 6	q - 26	l - 46	6 - 66	q - 86	l - 106	6 - 126
7 - 7	r - 27	m - 47	7 - 67	r - 87	m - 107	7 - 127
8 - 8	s - 28	n - 48	8 - 68	s - 88	n - 108	8 - 128
9 - 9	t - 29	o - 49	9 - 69	t - 89	o - 109	9 - 129
a - 10	u - 30	p - 50	a - 70	u - 90	p - 110	a - 130
b - 11	v - 31	q - 51	b - 71	v - 91	q - 111	
c - 12	w - 32	r - 52	c - 72	w - 92	r - 112	
d - 13	x - 33	s - 53	d - 73	x - 93	s - 113	
e - 14	y - 34	t - 54	e - 74	y - 94	t - 114	
f - 15	a - 35	u - 55	f - 75	a - 95	u - 115	
g - 16	b - 36	v - 56	g - 76	b - 96	v - 116	
h - 17	c - 37	w - 57	h - 77	c - 97	w - 117	
i - 18	d - 38	x - 58	i - 78	d - 98	x - 118	
j - 19	e - 39	y - 59	j - 79	e - 99	y - 119	

The ".eps" file

- NuShellX Will automatically generate simple level scheme diagrams in the encapsulated post script format.
- You need an eps viewing program to display these diagrams.
  - There is a freeware viewer called "gsview" you can download.
- On the right the diagram in the file "ne20w.eps" is shown.
- The length of the line is proportional to the angular momentum of the state.
  - The angular momentum and parity is labeled only for the lowest level of that angular momentum.
  - The color of the line indicates parity.
- The experimental values come from a database included with NuShellX.
  - I do not know what data is in this database or when it was last updated.
  - It is recommended that this data be used only as a qualitative guide.
  - Numerical values can be found in the file: "ne20exp.lpt"



M1 and E2 transition in ^{20}Ne

- We have already calculated the wave functions and energies we need for this example.
- The following inputs could have been appended to our previous inputs in shell.
- To begin type: “shell”
  - Make sure you are still in the directory with the previous output.
- We will make a batch script with a different name: “ne20t”
  - We could overwrite our previous script but we will keep it for completeness.
- We are interested in one body transition densities: “t”
  - Note we can also calculate 2 body transition densities and spectroscopic factors.
- We need to specify the file name that contains the initial state: “bw2400”
  - Note: the final 2 characters are modified by shell when we specify later arguments.
  - It should always be safe to end the file name with “00”.

M1 and E2 transition in ^{20}Ne

- We are interested in only one initial state. “1”
  - This is one state for a given angular momentum value.
- We need to specify the file for the final state. “bw2400”
  - Once again the final two characters will be modified by later input.
- We will calculate 5 final states per angular momentum value:”5”
- We are interested in only states with J=0 and J=2: 0,2,2
- Again: 0,2,2.
  - At this point shell has enough information to find the desired wave function overlap files.
- We wish to restrict the tensor ranks because we are interested only in E1 and M2 transitions:”y”
- For the M1 and E2 transitions: “1,2”
- We have everything we need: “st”
- Run the batch file by entering: “ne20t”

The ".deo" file

- After the calculation has run the human readable summary file is output to the current directory:
  - In our test case it is: ne200w.deo.
  - This file has all the details relevant to gamma decay.
  - There is another file that has simpler formatting and some different information with the extension ".dei". We will not discuss this in detail.
- The output is arranged by blocks of initial states.
  - Initial state information is in a single row at the start of a block.

```
gamma decay for ne200w.deo       BR greater than  0.000

! model space = sd
! interaction = w
! e_p =   1.360    e_n =   0.450   E2
! g_sp =  4.940    g_sn = -3.380   M1 spin
! g_lp =  1.137    g_ln = -0.079   M1 orbital
! g_pp =  0.340    g_pn = -0.220   M1 tensor

     Ei       Ji   ni         tau          T_(1/2)      M1 moment   Q moment        width
    (MeV)                    (psec)         (psec)       (u_N)    (e^2 fm^2)       (eV)

    1.776      2+    1       0.937990      0.650168      1.081       -14.29  -----  0.7015E-03

            Ef      Jf   nf    BR      Eg        del     B(1)         B(2)          A_p      A_n
            0.000    0+   1 100.0000  1.776   999.00   0.0000E+00  0.4924E+02      8.666    8.666

    7.316      2+    2       0.042574      0.029511      1.081       -14.29  -----  0.1546E-01

            Ef      Jf   nf    BR      Eg        del     B(1)         B(2)          A_p      A_n
            0.000    0+   1   1.2524  7.316   999.00   0.0000E+00  0.1145E-01      0.132    0.132
            1.776    2+   1  98.7476  5.540     9.31   0.8845E-04  0.3585E+01      2.339    2.339
```

The ".deo" file

- The lines of initial state information start in the leftmost column and include the following information.
  - Initial energy
  - Initial angular momentum
  - Index of initial state
  - Meant Lifetime
  - M1 moment
  - Q moment
  - Width

Ei (MeV)	Ji	ni	tau (psec)	T_(1/2) (psec)	M1 moment (u_N)	Q moment (e^2 fm^2)		width (eV)
1.776	2+	1	0.937990	0.650168	1.081	-14.29	-----	0.7015E-03

Ef	Jf	nf	BR	Eg	del	B(1)	B(2)	A_p	A_n
0.000	0+	1	100.0000	1.776	999.00	0.0000E+00	0.4924E+02	8.666	8.666

7.316	2+	2	0.042574	0.029511	1.081	-14.29	-----	0.1546E-01

Ef	Jf	nf	BR	Eg	del	B(1)	B(2)	A_p	A_n
0.000	0+	1	1.2524	7.316	999.00	0.0000E+00	0.1145E-01	0.132	0.132
1.776	2+	1	98.7476	5.540	9.31	0.8845E-04	0.3585E+01	2.339	2.339

The ".deo" file

- The lines of final state information start in the second column and include the following information.
  - final energy
  - final angular momentum
  - Index of final state
  - Branching Ratio
  - Energy of the gamma
  - del
  - B(M1)
  - B(E2)
  - A_p
  - A_n

Ei (MeV)	Ji	ni	tau (psec)	T_(1/2) (psec)	M1 moment (u_N)	Q moment (e^2 fm^2)		width (eV)
1.776	2+	1	0.937990	0.650168	1.081	-14.29	-----	0.7015E-03

Ef	Jf	nf	BR	Eg	del	B(1)	B(2)	A_p	A_n
0.000	0+	1	100.0000	1.776	999.00	0.0000E+00	0.4924E+02	8.666	8.666

Ei (MeV)	Ji	ni	tau (psec)	T_(1/2) (psec)	M1 moment (u_N)	Q moment (e^2 fm^2)		width (eV)
7.316	2+	2	0.042574	0.029511	1.081	-14.29	-----	0.1546E-01

Ef	Jf	nf	BR	Eg	del	B(1)	B(2)	A_p	A_n
0.000	0+	1	1.2524	7.316	999.00	0.0000E+00	0.1145E-01	0.132	0.132
1.776	2+	1	98.7476	5.540	9.31	0.8845E-04	0.3585E+01	2.339	2.339