UNIVERSITY OF SURREY

Shell Model Calculations (with NuShellX@MSU)

TALENT Course 6
Theory for exploring nuclear reaction experiments

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Session outline

- A brief theoretical overview of the shell model
  - References
  - Central potential and residual interactions
  - General calculation procedure
- Examples of calculations
  - Levels and overlaps, what output is given
- A practical guide to shell model calculations
  - Interactions, models spaces
  - Truncations
  - Pitfalls…
- Overview of NuShellX@MSU calculations
  - Levels and overlaps

<u>Tutorial</u>

- Introduction and setup
- Proton spectroscopic factors: ^{26}Ne(-1p) [or ^{26}Ne(d,^{3}He)^{25}F]

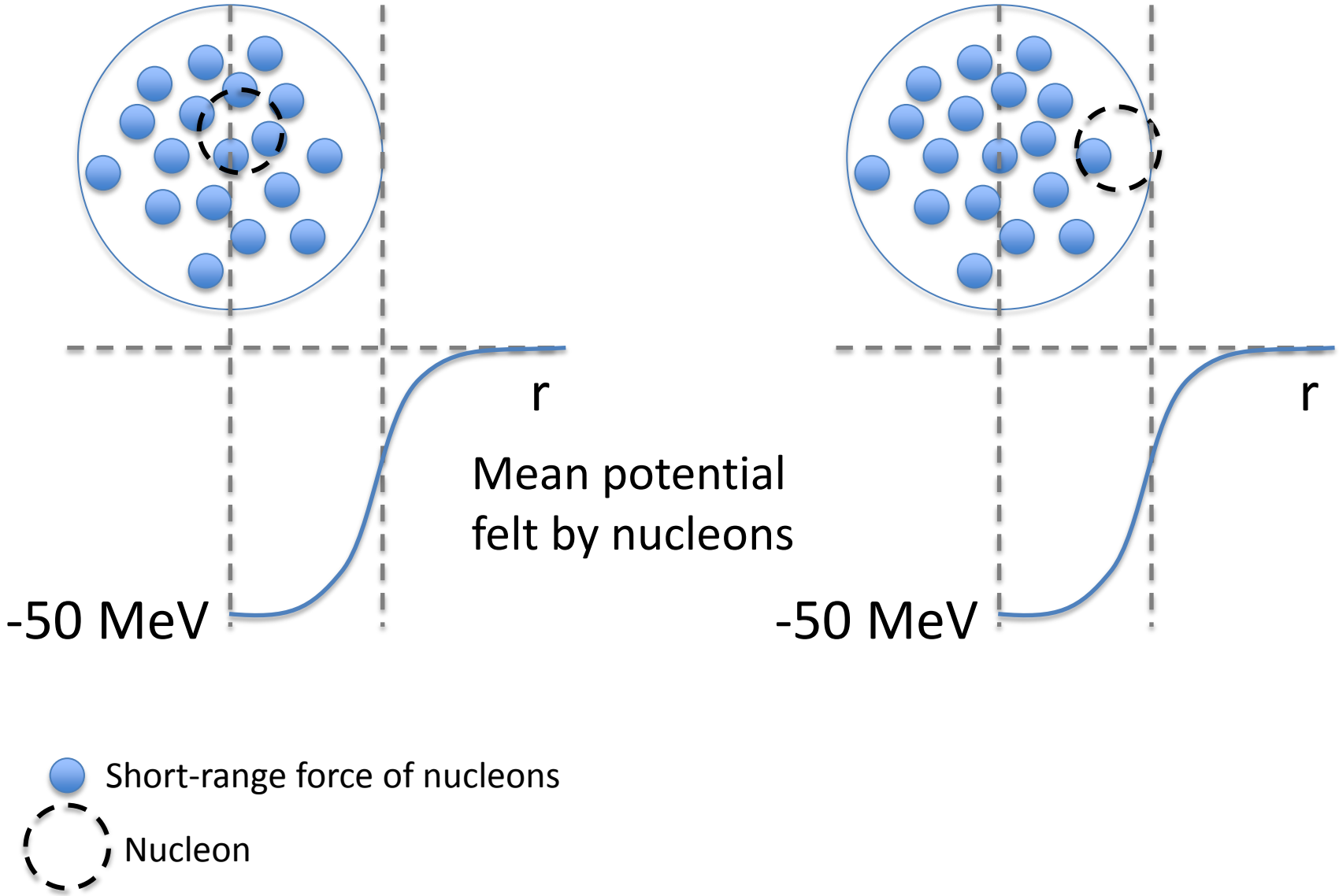
A brief overview of the shell model

Central potentials and residual interactions

References

1. H. Grawe, *Shell Model from a Practioner's Point of View*, Euroschool Lectures Vol. 1
2. T. Otsuka, Shell Structure of Exotic Nuclei, Euroschool Lectures Vol. 2
3. J. B. McGrory and B. H. Wildenthal, Ann. Rev. Nucl. Part. Sci. 30, 383 (1980)
4. B. A. Brown, *Lecture Notes in Nuclear Structure Physics* (2010)
5. Amos de-Shalit and Igal Talmi, *Nuclear Shell Theory*
6. M. Vallieres and H. Wu, in *Computational Nuclear Physics I: Nuclear Structure*
7. E. Caurier and F. Nowacki, *Act. Phys. Pol. B 30, 705 (1999)*

Mean potential from NN interactions



In a Nu(t)shell

- Shell-model Hamiltonian written as:

$$H = T + V = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i>k=1}^{A} V_{ik}(r_1, r_2)$$

- Three-body interaction small enough at energies of interest such that effects are absorbed into effective two-body interaction

$$H = T + V = \sum_{i=1}^{A} \left[\frac{p_i^2}{2m} + U_i(\vec{r}) \right] + \sum_{i>k=1}^{A} V_{ik}(r_1, r_2) - \sum_{i=1}^{A} U_i(\vec{r})$$

$$H = H_0 + H_{12}$$

- Absorb most of the effects of the two-body interactions into a one-body central potential

The shell model

- We wish to solve find the eigenstates and eigenvalues (energies) of the Hamiltonian *H*

$$H \left| \Psi_{\alpha} \right\rangle = E \left| \Psi_{\alpha} \right\rangle$$

- Solutions of the central part H_0 are products of single particle wave functions

$$H_0 \left| \Phi_{\alpha} \right\rangle = E_{\alpha} \left| \Phi_{\alpha} \right\rangle \qquad \left| \Phi_{\alpha} \right\rangle = \left| \phi_1 \right\rangle \left| \phi_2 \right\rangle \left| \phi_3 \right\rangle \ldots \left| \phi_N \right\rangle$$

- The solution requires matrix elements of *H:*

$$\left\langle \Phi_{\alpha} \left| H \right| \Phi_{\beta} \right\rangle$$

- The matrix elements of the central part may be calculated using an assumed potential or related to single-particle energies

McGrory and Wildenthal (1980)

The shell model

- Any *n*-particle shell model matrix element can be reduced to a linear combination of two-particle matrix elements:

$$\left\langle \Phi_\alpha \left| H_{12} \right| \Phi_\beta \right\rangle = \sum_{i,j,k,l,J,T} C_{\alpha\beta}^{ijklJT} \left\langle ijJT \left| H_{12} \right| klJT \right\rangle$$

- Form a matrix of H and then diagonalize:

$$H = \begin{bmatrix} \langle \Phi_1 | H | \Phi_1 \rangle & \langle \Phi_1 | H | \Phi_2 \rangle & * & * & * & . & . \\ \langle \Phi_2 | H | \Phi_1 \rangle & \langle \Phi_2 | H | \Phi_2 \rangle & * & * & . & . & . \\ \langle \Phi_3 | H | \Phi_1 \rangle & * & * & . & . & . & . \\ * & * & . & . & . & . & . \\ * & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{bmatrix} \xrightarrow{Diagonalis\ \ e} \begin{bmatrix} E_1 & & & & & & \\ & E_2 & & & & & \\ & & E_3 & & & & \\ & & & E_4 & & & \\ & & & & . & & \\ & & & & & . & \\ & & & & & & . \end{bmatrix}$$

The shell model

- With the matrix diagonalised we have solved for the eigenvectors and values $$H \left| \Psi \right\rangle = E \left| \Psi \right\rangle$$

- The wave functions are given as linear combinations of products of single-nucleon wave functions

$$\Psi = c_1 \Phi_1 + c_2 \Phi_2 + c_3 \Phi_3 + c_4 \Phi_4 + \ldots$$

- Obtain the decomposition of each state in terms of single-particle wave functions (protons and neutrons, and the angular momentum couplings)

$$S = \frac{|< \Psi^A \omega J || a_k^+ || \Psi^{A-1} \omega' J' >|^2}{(2J+1)}$$

Generalised procedure [McGrory (1980)]

1. Choice of the central potential H_0
2. Calculation of one-particle eigenstates in the desired model space
3. Construction of multi-nucleon eigenstates of H_0 from one-particle eigenstates
4. Specification of the residual interaction H_{12}
5. Evaluation of the matrix elements of H_{12} between the multi-nucleon eigenstates of H_0, and the calculation of eigenvectors and eigenvalues of this matrix

McGrory and Wildenthal (1980)

Differences in approach

- Different codes use different approaches to basis construction:
  - m-scheme: basis states are eigenstates of J_z
  - jj-coupling: construction of antisymmetric N-particle states using coefficients of fractional parentage (CFPs):

$$\left[j^{N-1}(\alpha' J'),\ jJ \ |\} \ j^{N} \alpha J \right]$$

- Oxbash/NuShell/NuShellX use both m-scheme and jj-coupling
- NuShellX is pn-formalism: creates basis states for protons and neutrons separately
- Different procedures for diagonalization: very often the Lanczos algorithm used (finds lowest energy eigenvalues efficiently)

Examples of calculations

Protons in ^{26}Ne

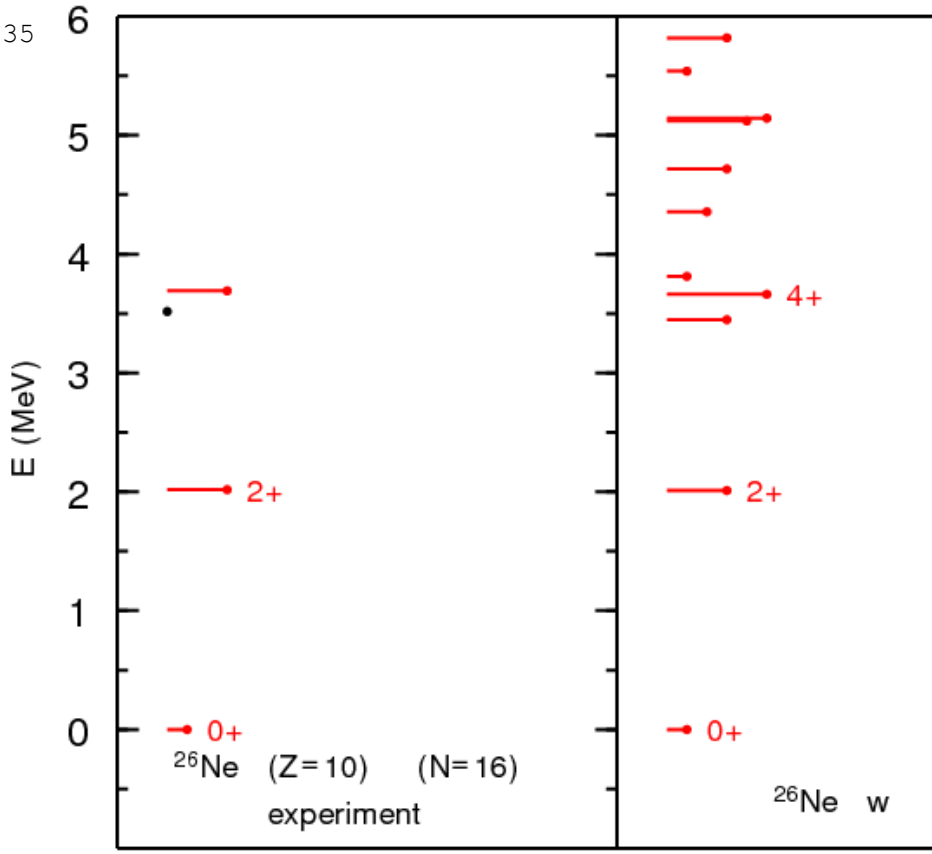
Neutrons in Calcium isotopes

Example: ^{26}Ne calculated level scheme and .lpe files

USD interaction in an sd-shell model space

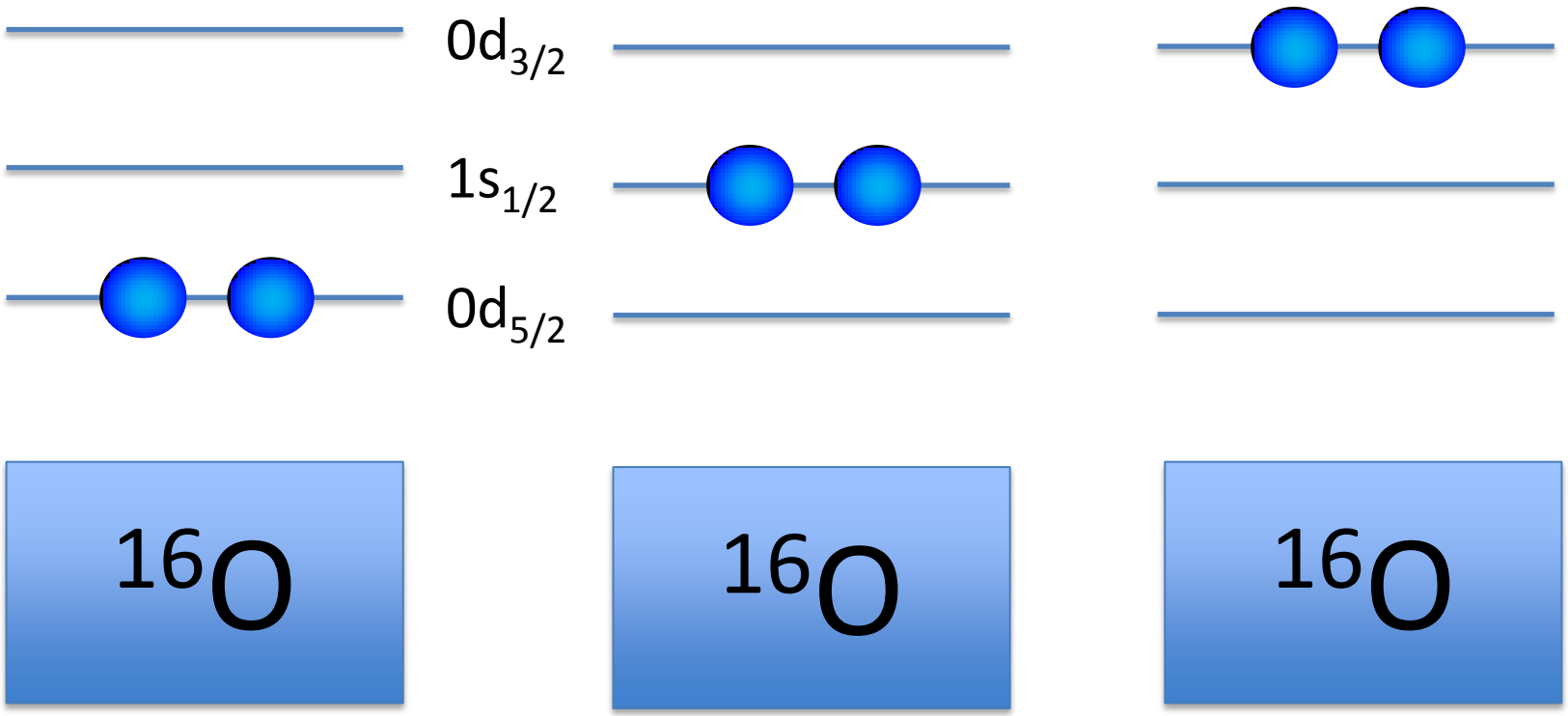
```
------------------------------------------------------------
a =  26 z = 10

Interaction file information from ne26w.mit
Interaction   spe-norm    tbme-norm  spe
w              1.00000      0.89555  1.6466 -3.9478 -3.1635
```

N	Njp	E(MeV)	Ex(MeV)	J	p	lowest Ex	name
1	1	-81.625	0.000	0	+	0.000	bw2a00.lpe
2	1	-79.614	2.011	2	+	2.011	bw2a04.lpe
3	2	-78.177	3.448	2	+		bw2a04.lpe
4	1	-77.963	3.662	4	+	3.662	bw2a08.lpe
5	2	-77.813	3.812	0	+		bw2a00.lpe
6	1	-77.269	4.356	1	+	4.356	bw2a02.lpe
7	3	-76.908	4.717	2	+		bw2a04.lpe
8	1	-76.505	5.120	3	+	5.120	bw2a06.lpe
9	2	-76.483	5.143	4	+		bw2a08.lpe
10	3	-76.086	5.539	0	+		bw2a00.lpe
11	4	-75.807	5.819	2	+		bw2a04.lpe
12	2	-75.569	6.056	3	+		bw2a06.lpe
13	5	-75.538	6.087	2	+		bw2a04.lpe
14	2	-75.415	6.210	1	+		bw2a02.lpe
15	1	-75.124	6.501	6	+	6.501	bw2a0c.lpe
16	6	-75.065	6.560	2	+		bw2a04.lpe
17	3	-74.876	6.749	3	+		bw2a06.lpe
18	7	-74.711	6.914	2	+		bw2a04.lpe
19	3	-74.602	7.023	4	+		bw2a08.lpe
20	4	-74.570	7.055	3	+		bw2a06.lpe
21	4	-74.368	7.257	0	+		bw2a00.lpe
22	3	-74.340	7.285	1	+		bw2a02.lpe
23	8	-74.197	7.428	2	+		bw2a04.lpe
24	1	-74.106	7.519	5	+	7.519	bw2a0a.lpe
25	4	-73.988	7.637	4	+		bw2a08.lpe
26	5	-73.949	7.676	3	+		bw2a06.lpe



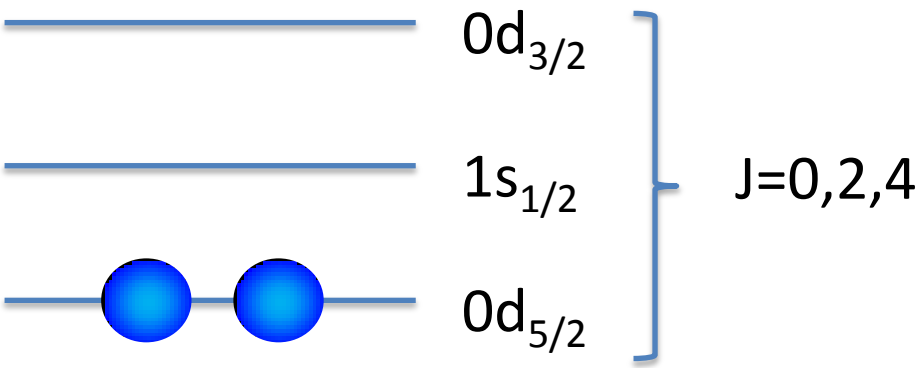
Partitions: distribution particles amongst orbits

Two-protons in an sd-shell model space

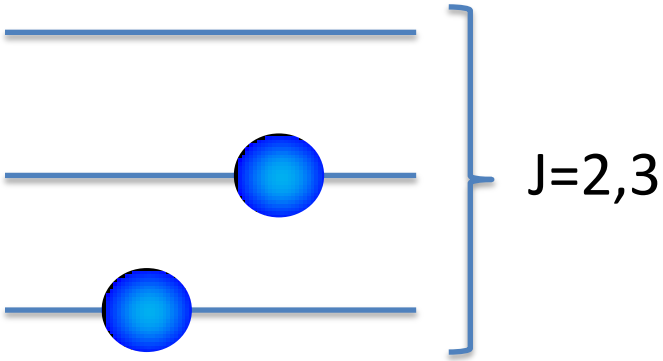


Angular momentum couplings of partitions

Two-protons in an sd-shell model space



^{16}O



^{16}O

Plus neutron configurations!

Example: ^{26}Ne levels (bw2a00.lpe)

Header Information

```
! ---------- shell input for bw2a00.lpe
sd                  input *.sp file name
sdpn                proton-neutron *.sp file
name
w                   interaction file name
 6          number of pn orbitals

  NuShellX V4.0 R2.003

  W.D.M. Rae, Garsington, Oxford 2008

  Uses NuShell code by W.D.M. Rae, Garsington,
Oxford, UK, 2006/7

   ne260s

  NuShellX is a nuclear shellmodel program
  written in Fortran95 for Windows/Linux.
  It is based on NuShell by W D M Rae 2007

  2*J,   2*T           0           6

  Lowest Energy Levels
```

List of Partitions

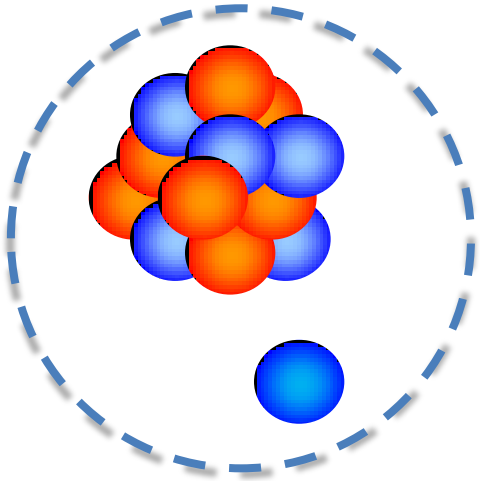
```
Type a = n  Type b = p
A partitions
    -1    0    0    0    4    4    0
    -2    0    0    0    3    5    0
    -3    0    0    0    2    6    0
    -4    0    0    0    4    3    1
    -5    0    0    0    3    4    1
    -6    0    0    0    2    5    1
    -7    0    0    0    1    6    1
    -8    0    0    0    4    2    2
    -9    0    0    0    3    3    2
   -10    0    0    0    2    4    2
   -11    0    0    0    1    5    2
   -12    0    0    0    0    6    2
B partitions
    -1    2    0    0    0    0    0
    -2    1    1    0    0    0    0
    -3    0    2    0    0    0    0
    -4    1    0    1    0    0    0
    -5    0    1    1    0    0    0
    -6    0    0    2    0    0    0
```

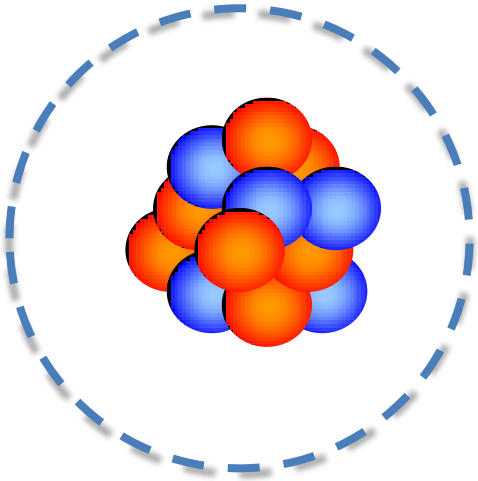
Example: ^{26}Ne levels (bw2a00.lpe)

Decomposition of each state

```
State            1  -81.62506      +

Average A type nucleons
  0.0000   0.0000   0.0000   0.7201   5.6681   1.6118

Average B type nucleons
  0.1341   1.6118   0.2540   0.0000   0.0000   0.0000
 Positive and Negative Parity
 +ve   100.00 % -ve     0.00%

 2*JA, 2*JB, amplitude            0           0   81.35678
 B partition, amplitude            1   4.801839
 A partitions, amplitudes
(  1,   0.03)(  2,   0.00)(  3,   0.49)(  4,   0.00)(  5,   0.01)(  6,   0.02)
(  7,   0.00)(  8,   0.02)(  9,   0.00)( 10,   0.54)( 11,   0.00)( 12,   3.68)
 B partition, amplitude            3   67.79593
 A partitions, amplitudes
(  1,   0.58)(  2,   0.00)(  3,   9.52)(  4,   0.00)(  5,   0.13)(  6,   0.17)
(  7,   0.00)(  8,   0.30)(  9,   0.02)( 10,   8.00)( 11,   0.00)( 12,  49.08)
 B partition, amplitude            6   8.759010
 A partitions, amplitudes
(  1,   0.07)(  2,   0.00)(  3,   1.11)(  4,   0.00)(  5,   0.02)(  6,   0.07)
(  7,   0.00)(  8,   0.03)(  9,   0.00)( 10,   0.88)( 11,   0.00)( 12,   6.58)

 2*JA, 2*JB, amplitude            4           4   16.04640
 B partition, amplitude            2   1.509106
 A partitions, amplitudes
(  1,   0.00)(  2,   0.09)(  3,   0.04)(  4,   0.01)(  5,   0.02)(  6,   0.13)
(  7,   0.44)(  8,   0.00)(  9,   0.03)( 10,   0.03)( 11,   0.71)( 12,   0.00)
 B partition, amplitude            3   6.580017
```

Spectroscopic factors for ^{26}Ne(-1p) -> ^{25}F





$(J_F M_F \; jm \mid J_{Ne} M_{Ne})$

$1/2^+, 3/2^+, 5/2^+$

^{25}F

^{26}Ne 0^+

$$S = \frac{|< \Psi^{A} \omega J || \overbrace{a_k^+}^{j} || \overbrace{\Psi^{A-1} \omega' J' >}^{^{25}F}|^2}{(2J+1)}$$

(^{26}Ne)

Examples: ^{26}Ne(-1p) SF Output (ne26w.lsf)

Initial=lighter, final=heavier

```
! model space = sd
! interaction = w
```

(Ai	Tzi)	(Af	Tzf)	(type	n,l,2j)	Ji	Jf	ni	nf	C^2S	Ei	Ef	C^2S*(Ef-Ei)	Exi	Exf
(25	3.5)	(26	3.0)	(p	2 0 1)	0.5+	0.0+	1	1	0.2427	-58.503	-81.625	-5.612	0.911	0.000
(25	3.5)	(26	3.0)	(p	2 0 1)	0.5+	0.0+	2	1	0.0001	-55.345	-81.625	-0.003	4.069	0.000
(25	3.5)	(26	3.0)	(p	2 0 1)	0.5+	0.0+	3	1	0.0081	-53.397	-81.625	-0.229	6.017	0.000
(25	3.5)	(26	3.0)	(p	2 0 1)	0.5+	0.0+	4	1	0.0004	-52.331	-81.625	-0.012	7.083	0.000
(25	3.5)	(26	3.0)	(p	2 0 1)	0.5+	0.0+	5	1	0.0004	-51.589	-81.625	-0.012	7.825	0.000
(25	3.5)	(26	3.0)	(p	2 0 1)	0.5+	0.0+	6	1	0.0006	-51.408	-81.625	-0.018	8.006	0.000
(25	3.5)	(26	3.0)	(p	2 0 1)	0.5+	0.0+	7	1	0.0000	-50.856	-81.625	0.000	8.558	0.000
(25	3.5)	(26	3.0)	(p	2 0 1)	0.5+	0.0+	8	1	0.0002	-49.672	-81.625	-0.006	9.742	0.000
(25	3.5)	(26	3.0)	(p	2 0 1)	0.5+	0.0+	9	1	0.0004	-49.475	-81.625	-0.013	9.939	0.000
(25	3.5)	(26	3.0)	(p	2 0 1)	0.5+	0.0+	10	1	0.0002	-48.821	-81.625	-0.007	10.593	0.000
									sum	0.2531			-5.911		

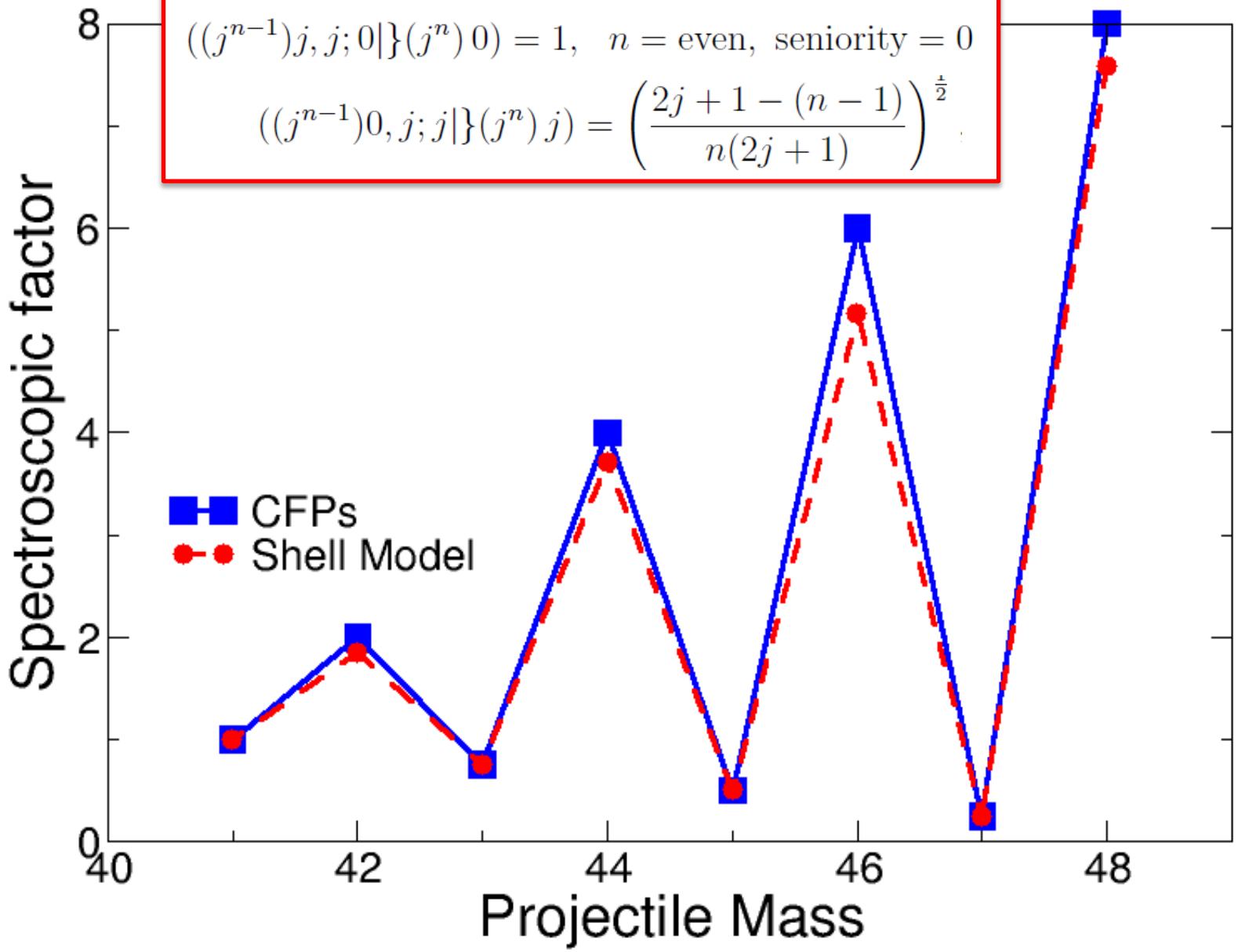
(Ai	Tzi)	(Af	Tzf)	(type	n,l,2j)	Ji	Jf	ni	nf	C^2S	Ei	Ef	C^2S*(Ef-Ei)	Exi	Exf
(25	3.5)	(26	3.0)	(p	1 2 3)	1.5+	0.0+	1	1	0.0300	-56.341	-81.625	-0.759	3.073	0.000
(25	3.5)	(26	3.0)	(p	1 2 3)	1.5+	0.0+	2	1	0.0507	-55.427	-81.625	-1.328	3.987	0.000
(25	3.5)	(26	3.0)	(p	1 2 3)	1.5+	0.0+	3	1	0.0355	-54.365	-81.625	-0.968	5.049	0.000
(25	3.5)	(26	3.0)	(p	1 2 3)	1.5+	0.0+	4	1	0.0034	-53.953	-81.625	-0.094	5.461	0.000
(25	3.5)	(26	3.0)	(p	1 2 3)	1.5+	0.0+	5	1	0.0003	-52.833	-81.625	-0.009	6.581	0.000
(25	3.5)	(26	3.0)	(p	1 2 3)	1.5+	0.0+	6	1	0.0003	-52.477	-81.625	-0.009	6.937	0.000
(25	3.5)	(26	3.0)	(p	1 2 3)	1.5+	0.0+	7	1	0.0054	-51.591	-81.625	-0.162	7.823	0.000
(25	3.5)	(26	3.0)	(p	1 2 3)	1.5+	0.0+	8	1	0.0038	-51.007	-81.625	-0.116	8.407	0.000
(25	3.5)	(26	3.0)	(p	1 2 3)	1.5+	0.0+	9	1	0.0002	-50.891	-81.625	-0.006	8.523	0.000
(25	3.5)	(26	3.0)	(p	1 2 3)	1.5+	0.0+	10	1	0.0000	-50.363	-81.625	0.000	9.051	0.000
									sum	0.1296			-3.451		

(Ai	Tzi)	(Af	Tzf)	(type	n,l,2j)	Ji	Jf	ni	nf	C^2S	Ei	Ef	C^2S*(Ef-Ei)	Exi	Exf
(25	3.5)	(26	3.0)	(p	1 2 5)	2.5+	0.0+	1	1	1.5665	-59.414	-81.625	-34.794	0.000	0.000
(25	3.5)	(26	3.0)	(p	1 2 5)	2.5+	0.0+	2	1	0.0203	-55.658	-81.625	-0.527	3.756	0.000
(25	3.5)	(26	3.0)	(p	1 2 5)	2.5+	0.0+	3	1	0.0095	-54.615	-81.625	-0.257	4.799	0.000
(25	3.5)	(26	3.0)	(p	1 2 5)	2.5+	0.0+	4	1	0.0001	-53.783	-81.625	-0.003	5.631	0.000
(25	3.5)	(26	3.0)	(p	1 2 5)	2.5+	0.0+	5	1	0.0051	-53.392	-81.625	-0.144	6.022	0.000
(25	3.5)	(26	3.0)	(p	1 2 5)	2.5+	0.0+	6	1	0.0004	-52.909	-81.625	-0.011	6.505	0.000
(25	3.5)	(26	3.0)	(p	1 2 5)	2.5+	0.0+	7	1	0.0000	-52.618	-81.625	0.000	6.796	0.000
(25	3.5)	(26	3.0)	(p	1 2 5)	2.5+	0.0+	8	1	0.0001	-51.380	-81.625	-0.003	8.034	0.000
(25	3.5)	(26	3.0)	(p	1 2 5)	2.5+	0.0+	9	1	0.0008	-51.228	-81.625	-0.024	8.186	0.000
(25	3.5)	(26	3.0)	(p	1 2 5)	2.5+	0.0+	10	1	0.0001	-51.016	-81.625	-0.003	8.398	0.000
									sum	1.6029			-35.766		
								total	sum	1.9856					

Examples: Calcium Isotopes (full fp-shell SM)

$$((j^{n-1})j, j; 0|\}(j^n)\,0) = 1, \quad n = \text{even}, \ \text{seniority} = 0$$

$$((j^{n-1})0, j; j|\}(j^n)\,j) = \left(\frac{2j+1-(n-1)}{n(2j+1)}\right)^{\frac{1}{2}}$$

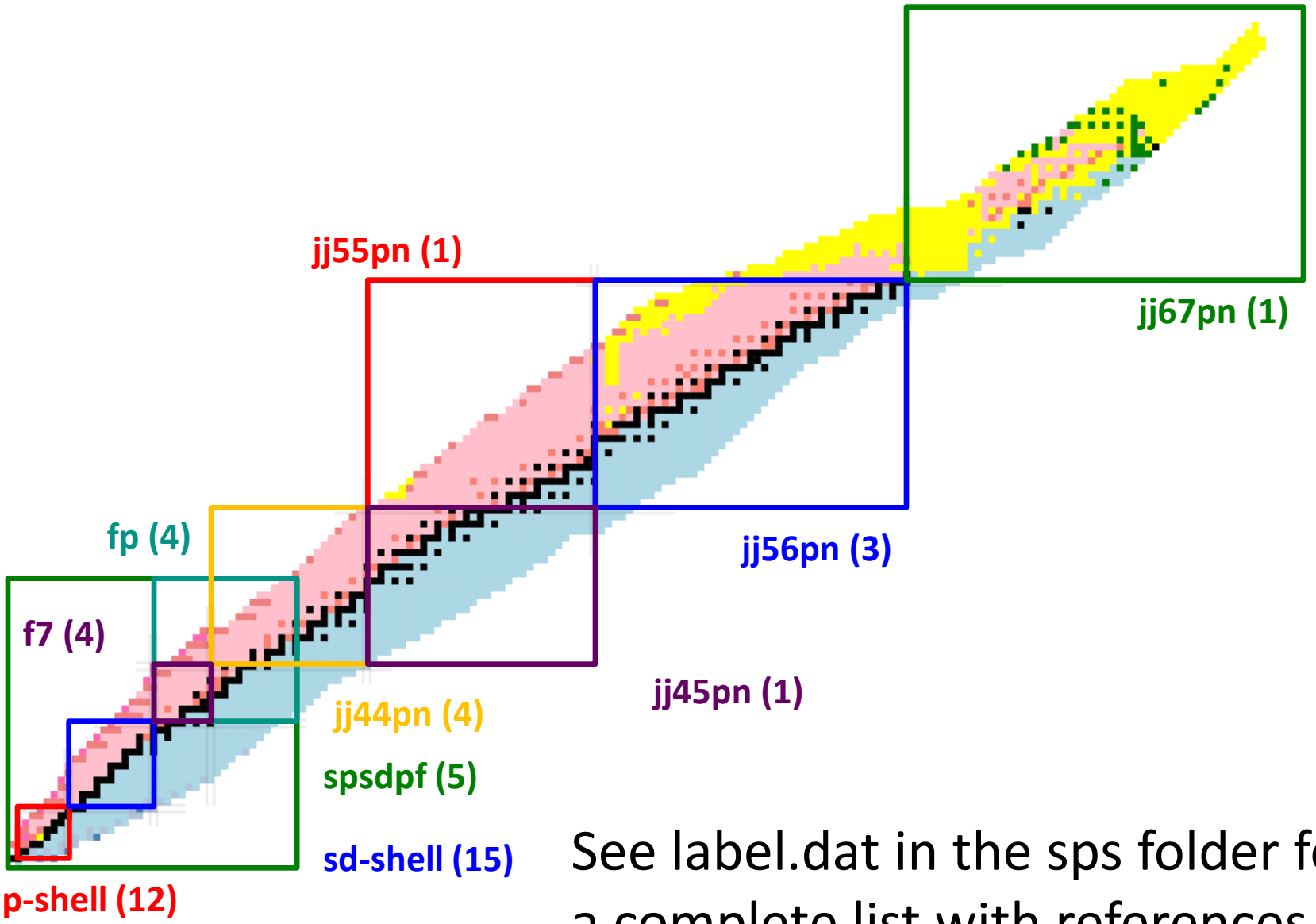


Model spaces, truncations and interactions

Model spaces

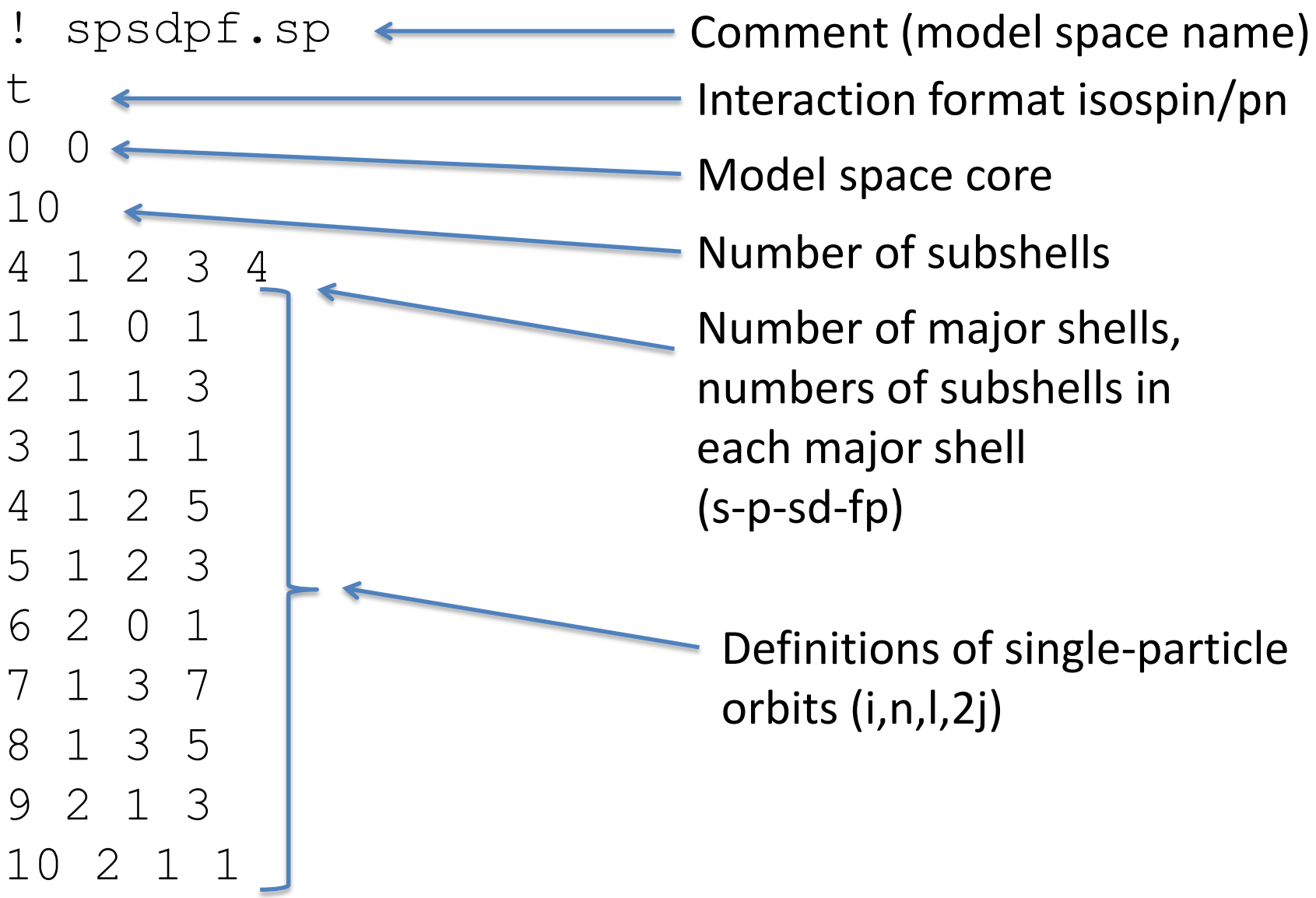
- Calculations in an infinite space are not possible – some truncation is required
- Model space defines the active valance nucleon orbits (two truncations, top and bottom)
- Generally, the best and most complete results are found with the largest model spaces
- … But the computation time increases exponentially with model space size…
- … And an the interaction used must be appropriate for the model space ...
- … And empirical interactions are (usually) better determined for smaller model spaces (fewer TBME)

(Some) Model Spaces



See label.dat in the sps folder for a complete list with references

Model spaces in NuShellX: .sp files



Residual Interactions

- Consist of a set of single particle energies and two-body matrix elements (TBME)
- Designed for a particular model space
  - BUT they may only be appropriate/feasible for a part of that model space
  - AND in model spaces crossing major shells the interaction may only be appropriate for a truncation of the (apparent) full model space

Origins of interactions

- Interactions are defined for a particular model space and consist of single-particle energies (SPE) and two-body matrix elements (TBME)
- Single-particle energies often taken from experiment, from the core + 1 nucleon nucleus
- The TBME are more complicated. Two methods are used:
  1. Empirical: either from phenomenological potentials or unconstrained fitting of TBME (but which states are included in the fit, is the solution unique, is it still predictive?)
  2. Realistic: TBME calculated using free nucleon-nucleon interaction
- Often a realistic interaction is used as a best first guess

Interactions in Oxbash/NuShellX

Comment (interaction details)

```
! The "USD" interaction of B. H. Wildenthal for A=18
! ORDER:  1 = 1D3/2    2 = 1D5/2    3 = 2S1/2
! The following spe give values of 15.63, 21.75 and 18.13 relative to
! 40Ca (1.612 -2.684 -2.967)
   63      1.6465800     -3.9477999     -3.1635399
  1   1   1   1         0   1     -2.1845000
  1   1   1   1         1   0     -1.4151000
  1   1   1   1         2   1     -0.0665000
  1   1   1   1         3   0     -2.8842001
  2   1   1   1         1   0      0.5647000
  2   1   1   1         2   1     -0.6149000
  2   1   1   1         3   0      2.0337000
  2   1   2   1         1   0     -6.5057998
  2   1   2   1         1   1      1.0334001
.....................
.............
.......
```

Number of TBME and single particle energies

Two-body matrix elements
o_1, o_2, o_3, o_4, J, T, TBME

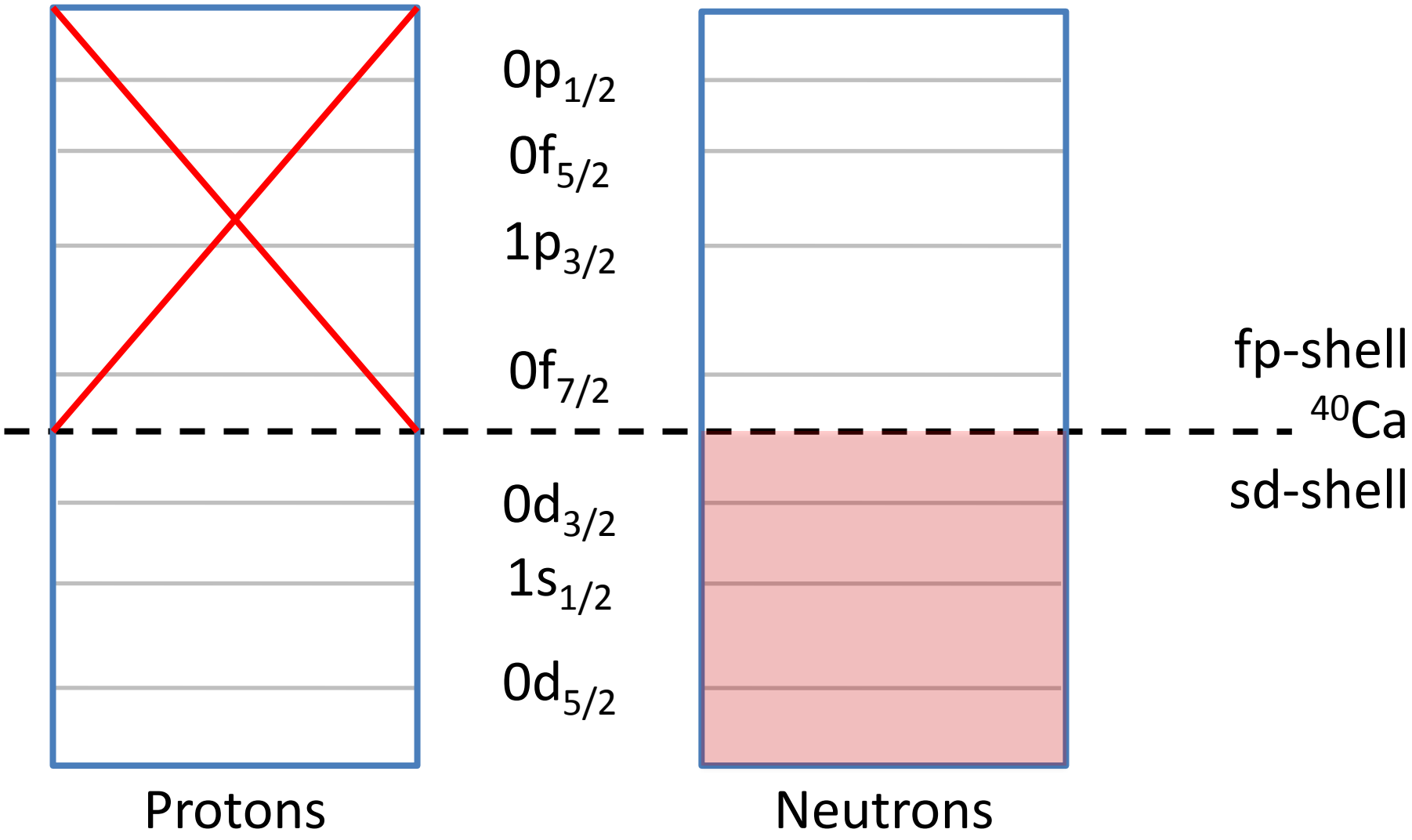
Isospin-formalism interactions automatically converted to pn-format

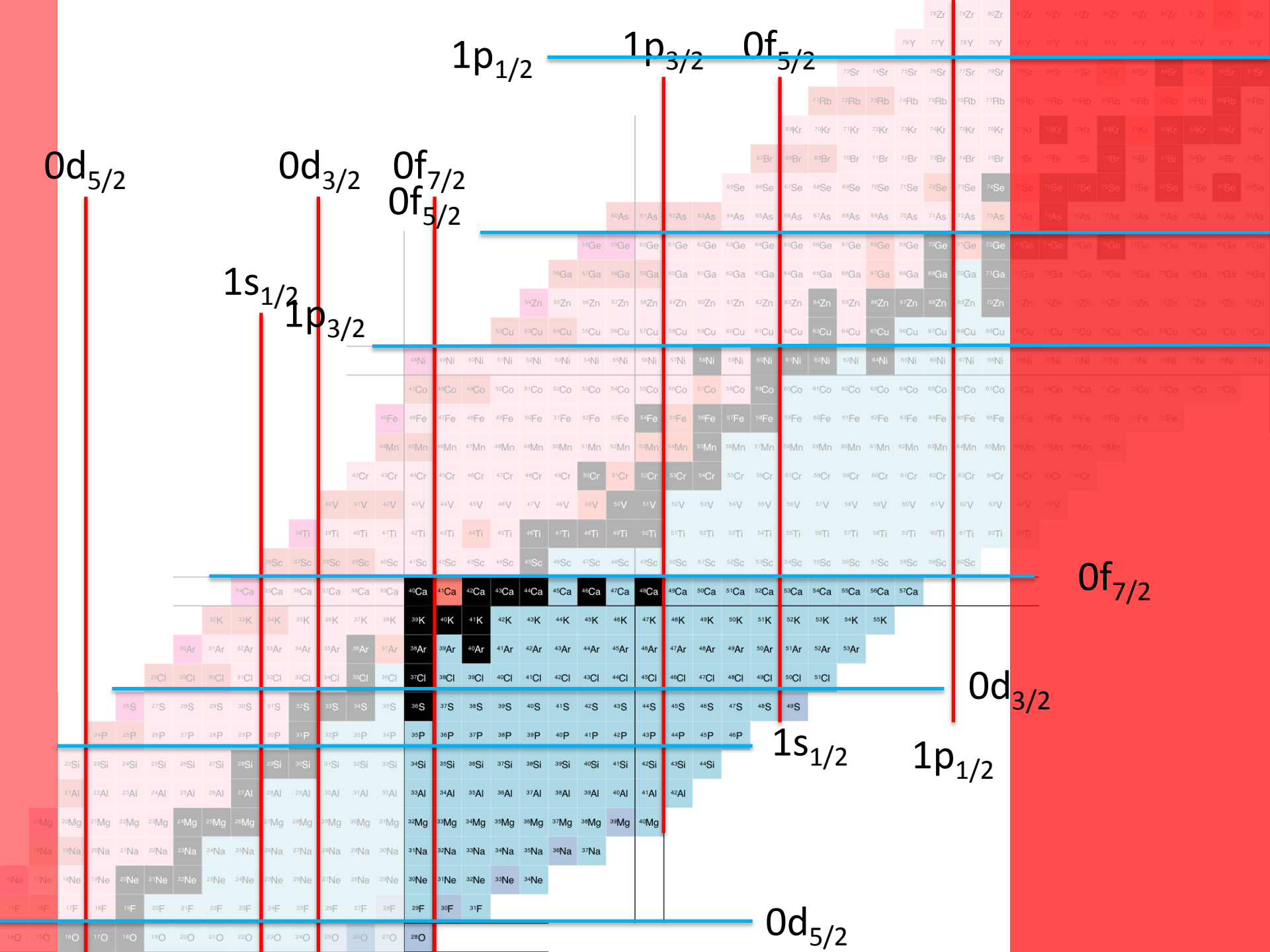
Model space truncations

- Calculations in the full model space may be too computationally intensive OR inappropriate for the interaction
- Truncate the model space to make calculations feasible
- Only subshell truncations are possible in NuShellX – limit numbers of protons (neutrons) in a given orbital
- Cannot restrict the total number of nucleons in a given orbital (proton and neutrons are treated separately)
- Truncations must be appropriate for interaction

Truncations – sdpf space

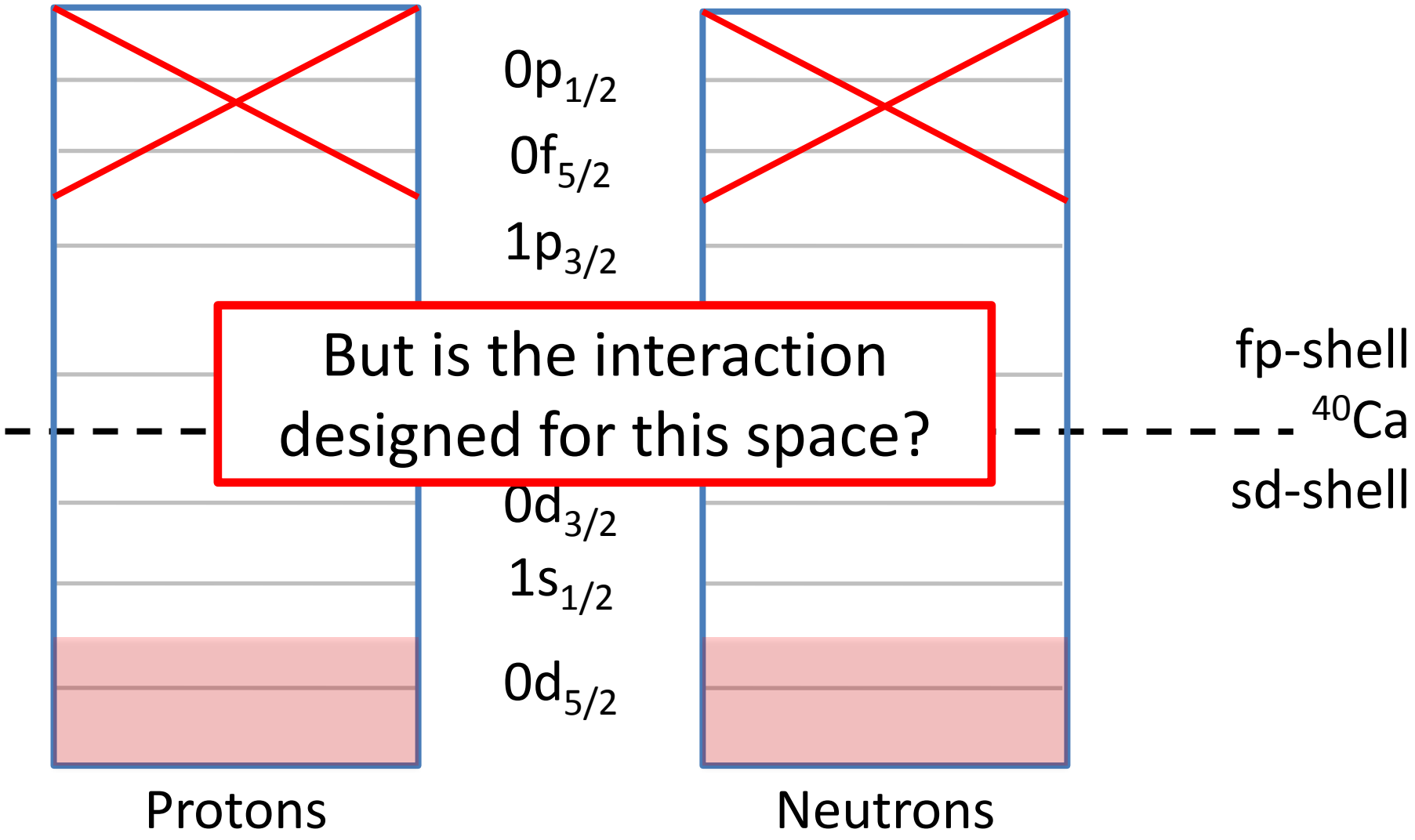
South-east of ^{40}Ca




1p1/2
1p3/2
0f5/2
0d5/2
0d3/2
0f7/2
0f5/2
1s1/2
1p3/2
0f7/2
0d3/2
1s1/2
1p1/2
0d5/2

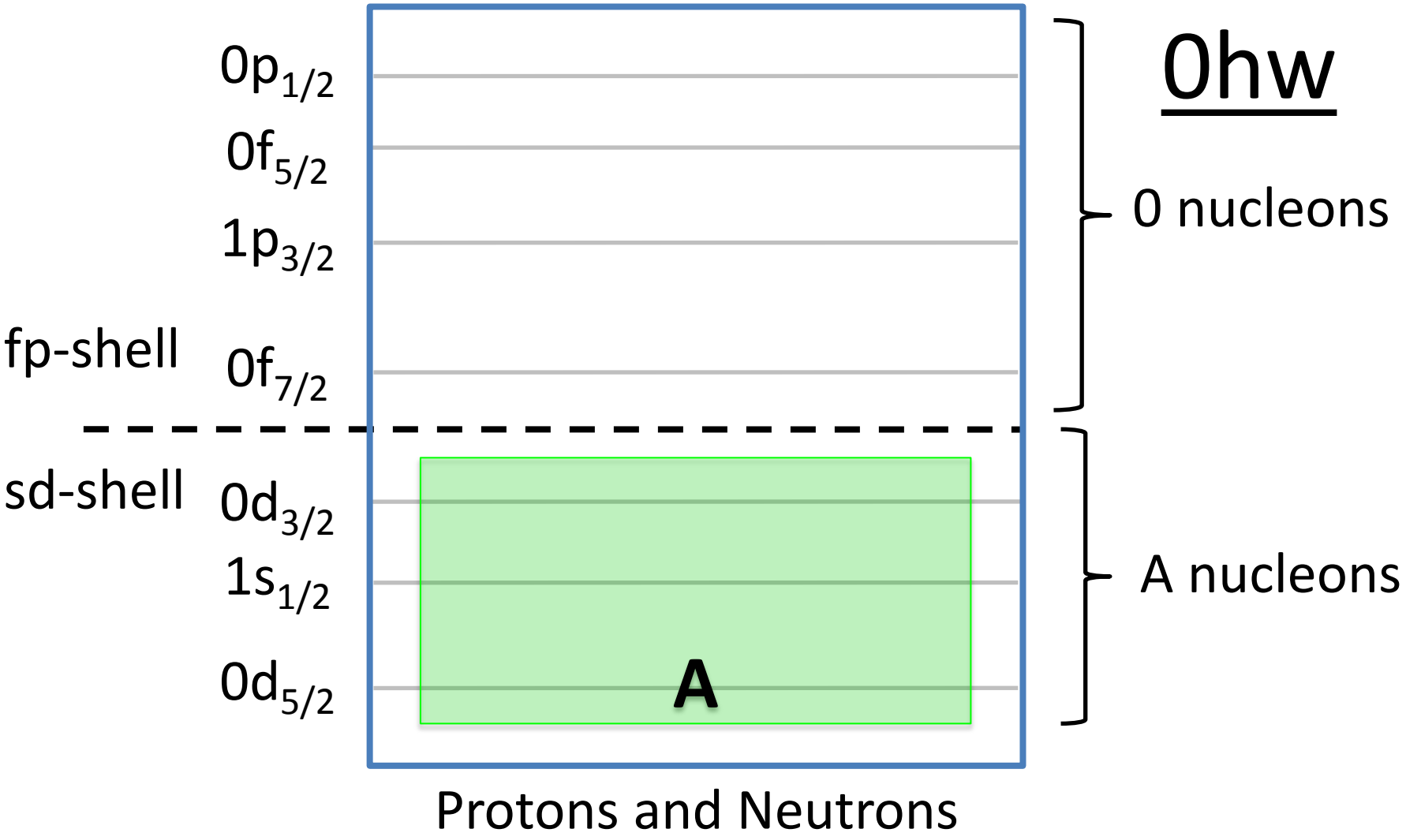
Truncations – sdpf space

Isotope shifts in $^{40\text{-}48}$Ca, $^{42\text{-}46}$Sc



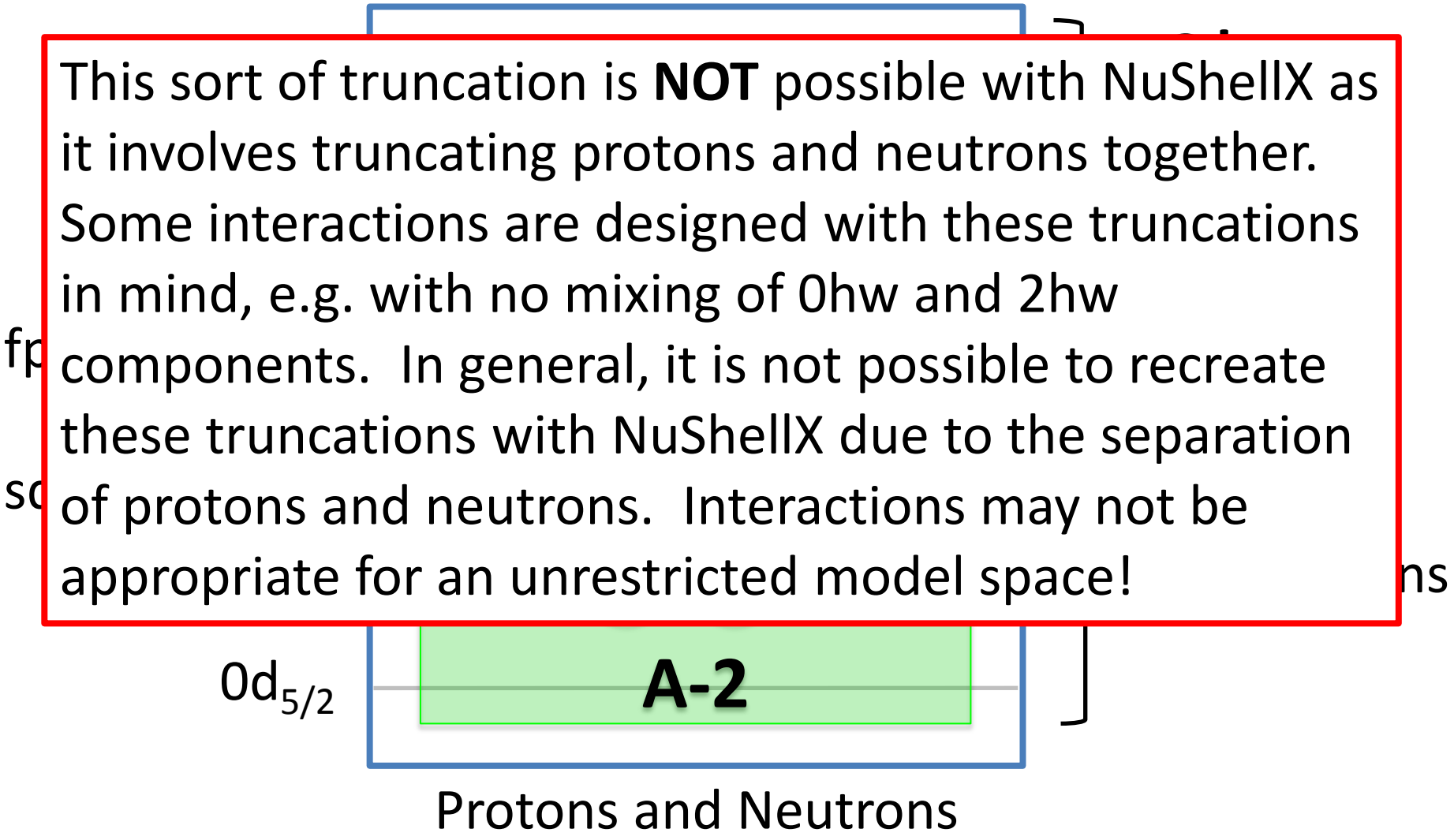
Truncations – hw (hbar-omega)

Number of excitations across a major shell gap



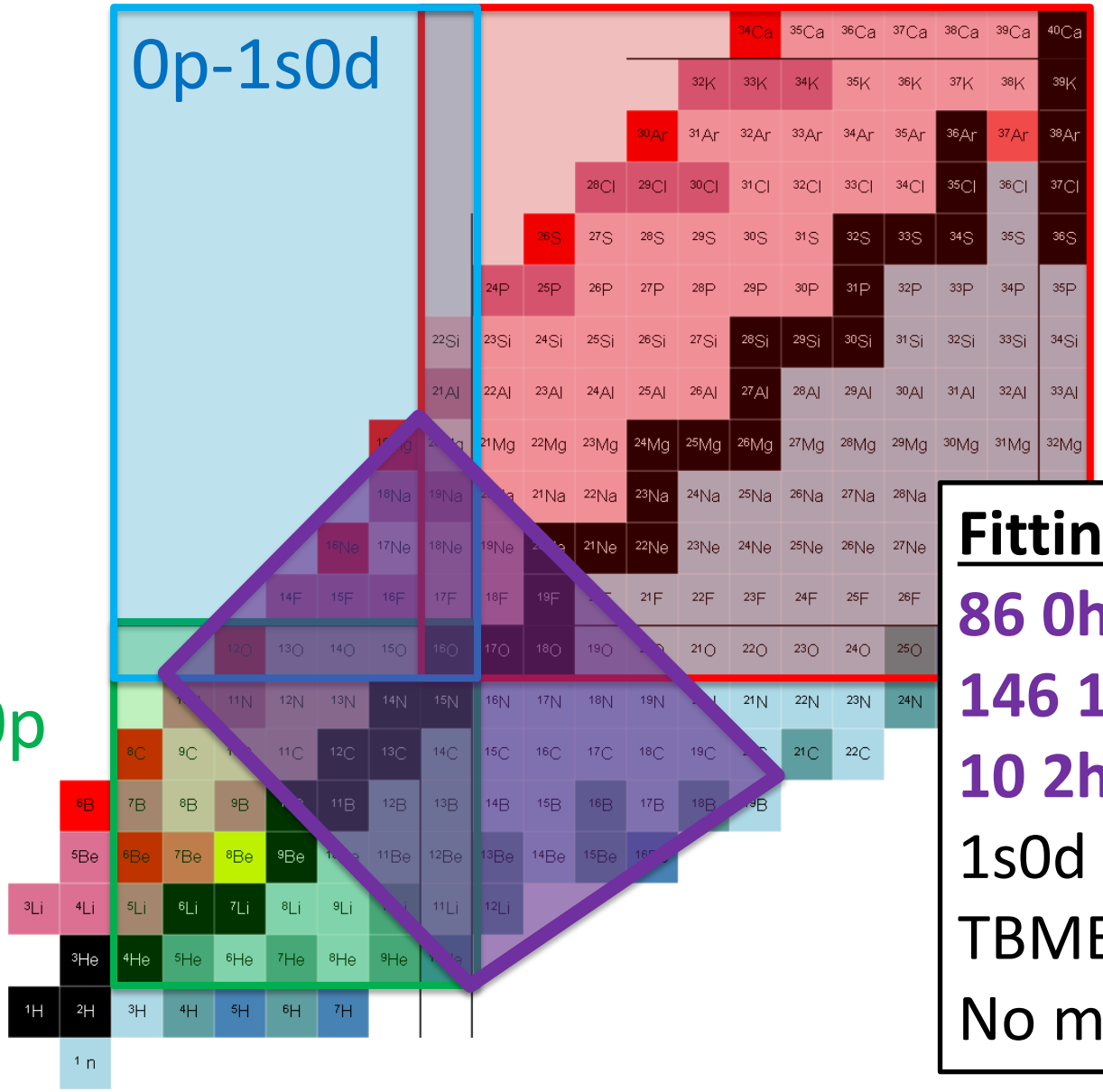
Truncations – hw (hbar-omega)

Number of excitations across a major shell gap



This sort of truncation is **NOT** possible with NuShellX as it involves truncating protons and neutrons together. Some interactions are designed with these truncations in mind, e.g. with no mixing of 0hw and 2hw components. In general, it is not possible to recreate these truncations with NuShellX due to the separation of protons and neutrons. Interactions may not be appropriate for an unrestricted model space!

Example: WBP/WBT interactions (p-sd)



Fitting

86 0hw (p-shell)

146 1hw

10 2hw

1s0d fixed USD

TBME of 0p, 0p-1s0d

No mixing of 0+2hw

Doing shell model calculations with NuShellX

History, setup, levels and overlaps

A brief history of Oxbash/NuShell/NuShellX

- Oxbash, W. D. M. Rae, B. A. Brown *et al.* (1976)
- NuShell ,W. D. M. Rae (2007)
- NuShellX, W. D. M. Rae (2008)
- NuShellX@MSU, B. A. Brown (2008)
- Provides an incredibly powerful tool for structure calculations, with enormously flexibility and freedom…
- BUT it is very easy to produce unrealistic or inappropriate calculations

More detail can be found in the NuShellX@MSU help.pdf file, located in X:/aaa/nushellx/help/

Doing shell model calculations

- Use (non-standard) command **`lab`** to open the file `label.dat`, located in `c:\TalentShare\aaa\nushellx\sps\`
- Choose appropriate model space
  - Several model spaces cover any given nuclide
  - How big does the model space need to be?
- Choose interaction
  - Can the calculations be done on your computer in the model space the interaction was designed for?
  - Similar published example for comparison/checking?
  - Recent
- Decide if model space truncations are required
  - Truncate appropriately for interaction
  - To begin, truncate severely – how good are simple calculations?
  - Relax truncations
- When publishing, give sufficient detail such that the calculations can be easily reproduced

Calculation of levels

- All calculations require levels
- Run **`shell`** and choose option **`lpe`**
- Enter the information requested
- Output of individual levels in **`.lpe`** files
- A summary of levels (calculated and experimental) in **`.lpt`** files

Calculating overlaps

- First calculate the levels (`.lpe`) of both the initial and final nuclei using **`shell`** option **`lpe`**
  - This must be done using the same model space and interaction
- Then calculate the overlaps of the form:

$$S = \frac{|< \Psi^A \omega J || a_k^+ || \Psi^{A-1} \omega' J' >|^2}{(2J+1)}$$

- All overlaps of the same general form
- Some [E(Lλ), M(L λ), B(GT)] then require calculations using **`dens`** – more info in the manual

Conclusions

- NuShellX@MSU is easy to use, but model spaces and interactions must be appropriately chosen
- Further information in help/help.pdf

Tutorial

- Run through sample calculation…
- Then tackle any problem you like