

# Introduction to NUSHELLX and transitions

Angelo Signoracci

CEA/Saclay

Lecture 4, 14 May 2013

# Outline

- 1 Introduction
- 2  $\beta$  decay
- 3 Electromagnetic transitions
- 4 Spectroscopic factors
- 5 Two-nucleon transfer/ other reaction model inputs

# Outline

- 1 Introduction
- 2  $\beta$  decay
- 3 Electromagnetic transitions
- 4 Spectroscopic factors
- 5 Two-nucleon transfer/ other reaction model inputs

# Review

- **Level schemes covered in Lecture III**

- 1 Calculate energies and wavefunctions with 'lpe' option of 'shell'
- 2 NUSHELLX provides output in \*.lp, \*.lpe, \*.lpt, and \*.eps files

- **From the wavefunction, can determine many properties of interest**

- 1  $\beta$  decay
- 2 Electromagnetic transitions
- 3 Spectroscopic information
- 4 ...

- Only need to know the appropriate operator

- Like the Hamiltonian, need effective operators in the reduced model space
- Requires consistent technique for all operators
- See Lecture VI for more information

- Typically, phenomenology guides operators in shell model

- For example, computation of electromagnetic transitions

Effective charges in the  $sd$  shell

$$e_p = 1.5e$$

$$e_n = 0.5e$$

# Review

- **Level schemes covered in Lecture III**

- 1 Calculate energies and wavefunctions with 'lpe' option of 'shell'
- 2 NUSHELLX provides output in \*.lp, \*.lpe, \*.lpt, and \*.eps files

- **From the wavefunction, can determine many properties of interest**

- 1  $\beta$  decay
- 2 Electromagnetic transitions
- 3 Spectroscopic information
- 4 ...

- **Only need to know the appropriate operator**

- Like the Hamiltonian, need effective operators in the reduced model space
- Requires consistent technique for all operators
- See Lecture VI for more information

- Typically, phenomenology guides operators in shell model

- For example, computation of electromagnetic transitions

Effective charges in the  $sd$  shell

$$e_p = 1.5e$$

$$e_n = 0.5e$$

# Review

- **Level schemes covered in Lecture III**

- ① Calculate energies and wavefunctions with 'lpe' option of 'shell'
- ② NUSHELLX provides output in \*.lp, \*.lpe, \*.lpt, and \*.eps files

- **From the wavefunction, can determine many properties of interest**

- ①  $\beta$  decay
- ② Electromagnetic transitions
- ③ Spectroscopic information
- ④ ...

- Only need to know the appropriate operator

- Like the Hamiltonian, need effective operators in the reduced model space
- Requires consistent technique for all operators
- See Lecture VI for more information

- **Typically, phenomenology guides operators in shell model**

- For example, computation of electromagnetic transitions

Effective charges in the  $sd$  shell

$$e_p = 1.5e$$

$$e_n = 0.5e$$

# One-body transition densities

- One-body transition densities (OBTD)
  - Provide the information to calculate matrix elements of one-body operators
  - Compact, convenient form
  - Different in  $J$ -scheme and  $m$ -scheme (only present  $J$ -scheme here)
  - Different in isospin and proton-neutron formalism (see Lecture 3 for definitions)
    - Only present simpler proton-neutron equations in lecture
- Given a one-body tensor operator of rank  $\lambda$

$$O^\lambda = \sum_{ij} \langle i | O^\lambda | j \rangle a_i^\dagger a_j$$

in a reduced model space with unique values of  $\ell, j$

- One-body transition densities between many-body states

$$\text{OBTD}(i, j, k, k', \lambda) = \sum_{k'' \in A-1} (-1)^{J_k + J_{k''} + \lambda - j} \left\{ \begin{matrix} J_{k'} & J_k & \lambda \\ j_i & j_j & J_{k''} \end{matrix} \right\} \\ \times \langle \Psi_k || a_i^\dagger || \Psi_{k''} \rangle \langle \Psi_{k'} || a_j^\dagger || \Psi_{k''} \rangle$$

- Product of  $6j$  coefficients and reduced matrix elements
- Related to coefficients of fractional parentage (CFP) (full derivation not included)

# One-body transition densities

- Write reduced matrix element between many-body states as a product of
  - 1 OBTD
  - 2 Reduced matrix elements between *single particle* states

$$\langle \Psi_k | \mathcal{O}^\lambda | \Psi_{k'} \rangle = \sum_{ij} \text{OBTD}(i, j, k, k', \lambda) \langle i || \mathcal{O}^\lambda || j \rangle$$

- Formalism looks complex, but greatly simplifies the many-body problem
- NUSHELLX calculates all OBTD between selected initial and final states
  - With 'den' option of 'shell'
  - In appropriate formalism (only proton-neutron shown here)
- Reduced single particle matrix elements
  - Calculated by 'dens' executable
  - Automatically run by NUSHELLX in many cases ( $B(E2)$ ,  $B(GT)$ , etc.)



# One-body transition densities

- Write reduced matrix element between many-body states as a product of
  - 1 OBTD
  - 2 Reduced matrix elements between *single particle* states

$$\langle \Psi_k | \mathcal{O}^\lambda | \Psi_{k'} \rangle = \sum_{ij} \text{OBTD}(i, j, k, k', \lambda) \langle i || \mathcal{O}^\lambda || j \rangle$$

- Formalism looks complex, but greatly simplifies the many-body problem
- **NUSHELLX calculates all OBTD between selected initial and final states**
  - With 'den' option of 'shell'
  - In appropriate formalism (only proton-neutron shown here)
- Reduced single particle matrix elements
  - Calculated by 'dens' executable
  - Automatically run by NUSHELLX in many cases ( $B(E2)$ ,  $B(GT)$ , etc.)

# One-body transition densities

- Write reduced matrix element between many-body states as a product of
  - 1 OBTD
  - 2 **Reduced matrix elements between *single particle states***

$$\langle \Psi_k | O^\lambda | \Psi_{k'} \rangle = \sum_{ij} \text{OBTD}(i, j, k, k', \lambda) \langle i || O^\lambda || j \rangle$$

- Formalism looks complex, but greatly simplifies the many-body problem
- NUSHELLX calculates all OBTD between selected initial and final states
  - With 'den' option of 'shell'
  - In appropriate formalism (only proton-neutron shown here)
- **Reduced single particle matrix elements**
  - Calculated by 'dens' executable
  - Automatically run by NUSHELLX in many cases ( $B(E2)$ ,  $B(GT)$ , etc.)

# Outline

- 1 Introduction
- 2  $\beta$  decay
- 3 Electromagnetic transitions
- 4 Spectroscopic factors
- 5 Two-nucleon transfer/ other reaction model inputs

# Introduction

- Primary method of decay for ground states of nuclei accessible with CI theory
  - $\beta^\pm$  decay converts a nucleus with  $(Z, A)$  to  $(Z \mp 1, A)$
  - $\beta^+$  decay can also proceed by electron capture (EC)
- Mediated by weak interaction in the form of  $W$  bosons
- Will only deal with so-called “allowed” decays
  - 1 No angular momentum carried away by electron and neutrino
  - 2 Not an actual selection rule- just dominant mode (by orders of magnitude)
  - 3 Two types: Fermi and Gamow-Teller decay
- $Q$ -value for  $\beta^\pm$  decay (ignoring electron binding energies)

$$BE(A, Z_f) - BE(A, Z_i) \mp \delta_{nH} - m_e c^2 x$$

where

$\delta_{nH} = 0.782 \text{ MeV}$     mass difference between neutron and Hydrogen atom

$x = 2$     for  $\beta^+$

$x = 0$     for electron capture and  $\beta^-$

# Fermi and Gamow-Teller decay

$$O(F_{\pm}) = \sum_{a=1}^A t_{a\pm}$$

$$O(GT_{\pm}) = \sum_{a=1}^A \sigma_a t_{a\pm}$$

$a$  index refers to all nucleons in the many-body system

- Fermi decay

- $\Delta S = 0$  ( $\Delta J = 0$ )

- $\Delta T = 0$  (recall from Lecture II: isospin treated as good quantum number)

$$\begin{aligned} B_{k,k'}(F_{\pm}) &= |\langle \Psi_k | O(F_{\pm}) | \Psi_{k'} \rangle|^2 \\ &= [T_k(T_k + 1) - T_{zk}(T_{zk} \pm 1)] \delta_{J_k J_{k'}} \delta_{M_k M_{k'}} \delta_{T_k T_{k'}} \end{aligned}$$

Only connects isobaric analogue states!

- Gamow-Teller decay

- $\Delta S = 1$  ( $\Delta J = 1$ )

- $\Delta T = 0, 1$  (isospin is good quantum number)

$$\begin{aligned} B_{k,k'}(GT_{\pm}) &= \frac{|\langle \Psi_k || O(GT_{\pm}) || \Psi_{k'} \rangle|^2}{2J_{k'} + 1} \equiv \frac{[M_{k,k'}(GT_{\pm})]^2}{2J_{k'} + 1} \\ &= \sum_{ij} \langle i || \sigma t_{\pm} || j \rangle \text{OBTD}(i, j, k, k', 1) \end{aligned}$$

$\beta^\pm$  decay

Half-life  $t_{1/2}$  typically quoted in terms of  $ft$  values given by

$$ft_{1/2}^{k,k'} = \frac{C}{B_{k,k'}(F_\pm) + (g_A/g_V)^2 B_{k,k'}(GT_\pm)}$$

where

$f$  = phase space factor depending on  $Q$ -value

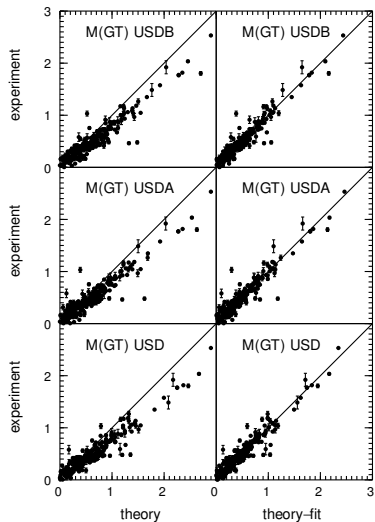
$C$  = constant with the value 6170(4)

$g_A$  = axial vector coupling constant

$g_V$  = vector coupling constant

- In QCD,  $g_A = -g_V$
- In nuclear physics, typically use value fit to neutron decay  $|g_A/g_V| = 1.261(8)$

# Comparison of experimental $M(GT)$ in $sd$ shell to empirical interactions<sup>1</sup>



- On left:
  - “bare” coupling constants
  - From neutron decay
- On right:
  - Least squares fit
  - As in QCD,  $|g_A/g_V| \approx 1$

<sup>1</sup>Courtesy of Alex Brown; from W.A. Richter et al., Phys. Rev. C **78**, 064302 (2008)

# Outline

- 1 Introduction
- 2  $\beta$  decay
- 3 Electromagnetic transitions**
- 4 Spectroscopic factors
- 5 Two-nucleon transfer/ other reaction model inputs



# Introduction

- Most common method of decay for low-lying excited states of nuclei
- Decay occurs within two states of same nucleus
- Mediated by electromagnetic interaction in the form of  $\gamma$  rays
- Sum of electric and magnetic multipole operators of tensor rank  $\lambda$

$$O = \sum_{\lambda\mu} [O(E\lambda)_\mu + O(M\lambda)_\mu]$$

$$O(E\lambda)_\mu = r^\lambda Y_\mu^\lambda(\hat{r}) e_{t_z}$$

$$O(M\lambda)_\mu = \sqrt{\lambda(2\lambda+1)} r^{\lambda-1} \mu_N \left[ \frac{2g_{t_z}^\ell}{\lambda+1} [Y^{\lambda-1} \otimes \vec{\ell}]_\mu^\lambda + g_{t_z}^s [Y^{\lambda-1} \otimes \vec{s}] \right]$$

- Free nucleon values:

$$e_p = 1 \quad g_p^\ell = 1 \quad g_p^s = 5.586$$

$$e_n = 0 \quad g_n^\ell = 0 \quad g_n^s = -3.826$$

## Reduced transitions

- As described above

$$\langle \Psi_k | O^\lambda | \Psi_{k'} \rangle = \sum_{ij} \text{OBTD}(i, j, k, k', \lambda) \langle i || O^\lambda || j \rangle$$

- Like the example for  $\beta$  decay, reduced matrix elements easy to find

$$\langle i || O(E\lambda) || j \rangle$$

$$\langle i || O(M\lambda) || j \rangle$$

- Calculated by 'dens' executable
- With the necessary selection rules, refer to reduced transition probability  $B$

$$B(X\lambda; k' \rightarrow k) = \frac{|\langle J_k || O(X\lambda) || J_{k'} \rangle|^2}{2J_{k'} + 1}$$

where

$$X = E \text{ or } M$$

## Reduced transitions

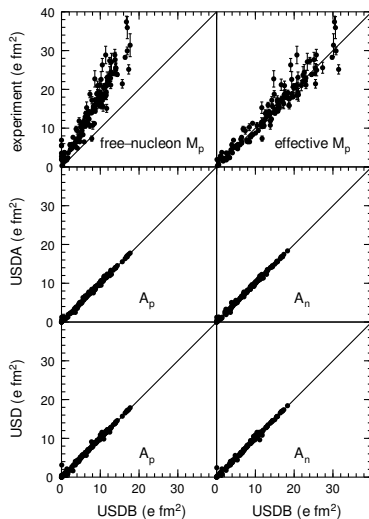
$$B(X\lambda; k' \rightarrow k) = \frac{|\langle \Psi_k || O(X\lambda) || \Psi_{k'} \rangle|^2}{2J_{k'} + 1} \equiv \frac{[M_{k,k'}(X\lambda)]^2}{2J_{k'} + 1}$$

- Reduced matrix element is symmetric between initial and final state
- Reduced transition probability depends on direction

$$B(X\lambda; k \rightarrow k') = \frac{2J_{k'} + 1}{2J_k + 1} B(X\lambda; k' \rightarrow k)$$

- Most common for shell model
  - $B(E2)$  (also provides quadrupole moment)
  - $B(M1)$  (also provides magnetic moment)
- Experimentally,  $B(E2)$  transitions are usually published
  - For Coulomb excitation:  $B(E2; \uparrow) \equiv B(E2; 0_1^+ \rightarrow 2_1^+)$
  - For  $\gamma$  decay:  $B(E2; \downarrow) \equiv B(E2; 2_1^+ \rightarrow 0_1^+)$

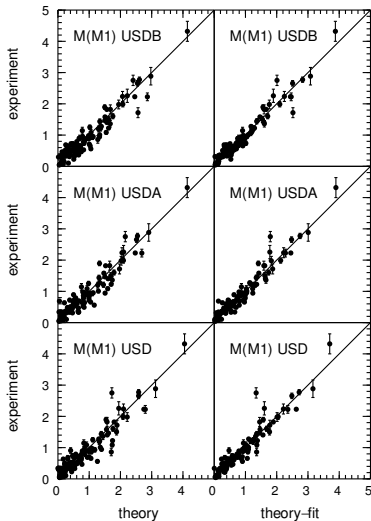
# Comparison of experimental $M(E2)$ in $sd$ shell to empirical interactions<sup>2</sup>



- Phenomenological effective charges for the  $sd$  shell ( $e_p \approx 1.5e$ ,  $e_n \approx 0.5e$ )

<sup>2</sup>Courtesy of Alex Brown; from W.A. Richter et al., Phys. Rev. C **78**, 064302 (2008)

# Comparison of experimental $M(M1)$ in $sd$ shell to empirical interactions<sup>3</sup>



- On left:
  - Free nucleon  $g$ -factors
- On right:
  - Least squares fit
  - $g_p^l = 1.16, g_n^l = -0.09$
  - $g_p^s = 5.15, g_n^s = -3.55$
  - Less affected than charge

<sup>3</sup>Courtesy of Alex Brown; from W.A. Richter et al., Phys. Rev. C **78**, 064302 (2008)

# Outline

- 1 Introduction
- 2  $\beta$  decay
- 3 Electromagnetic transitions
- 4 Spectroscopic factors**
- 5 Two-nucleon transfer/ other reaction model inputs

# Spectroscopic factors

- **Common notation- not employed by NUSHELLX**
- Briefly mentioned in Lecture 1 before developing formalism
- **Basis-independent, but not observable**
- Spectroscopic probability matrices

$$S_k^{+ij} \equiv \langle \Psi_0^A | a_i | \Psi_k^{A+1} \rangle \langle \Psi_k^{A+1} | a_j^\dagger | \Psi_0^A \rangle$$

and

$$S_{k'}^{-ij} \equiv \langle \Psi_0^A | a_j^\dagger | \Psi_{k'}^{A-1} \rangle \langle \Psi_{k'}^{A-1} | a_i | \Psi_0^A \rangle$$

- Spectroscopic factors found from tracing spectroscopic probability matrices
- In reduced model space, recover typical “definitions”

$$SF_k^+ \equiv |\langle \Psi_k^{A+1} | a_i^\dagger | \Psi_0^A \rangle|^2$$

and

$$SF_{k'}^- \equiv |\langle \Psi_{k'}^{A-1} | a_j | \Psi_0^A \rangle|^2$$

## Effective single particle energies (ESPE)

- Common notation- not employed by NUSHELLX
- Basis-independent, but not observable
- Requires summation over particle and hole states as described by Baranger<sup>4</sup>
- Solution to eigenvalue problem  $h^{cent} \psi_i^{cent} = e_i^{cent} \psi_i^{cent}$ , where

$$h_{ij}^{cent} \equiv \sum_{k \in \mathcal{H}_{A+1}} S_k^{+ij} (E_k^{A+1} - E_0) + \sum_{k \in \mathcal{H}_{A-1}} S_k^{-ij} (E_0 - E_k^{A-1})$$

- In reduced model space, recover

$$e_i^{cent} = \epsilon = \sum_{k \in \mathcal{H}_{A+1}} SF_k^+ (E_k^{A+1} - E_0) + \sum_{k \in \mathcal{H}_{A-1}} SF_k^- (E_0 - E_k^{A-1})$$

- Are ESPE observable? Can they be defined in absolute terms?<sup>5</sup>

<sup>4</sup>M. Baranger, Nucl. Phys. A **149**, 225 (1970)

<sup>5</sup>See T. Duguet and G. Hagen, Phys. Rev. C **85**, 034330 (2012)



# Notation in NUSHELLX

- Written explicitly with dependence on isospin

$$C^2 S_k^+ = |\langle TT_z | T' T'_z t t_z \rangle|^2 \frac{|\langle \Psi_k^{A+1} || a_i^\dagger || \Psi_{k'}^A \rangle|^2}{(2J+1)(2T+1)}$$

$$C^2 S_k^- = |\langle TT_z | T' T'_z t t_z \rangle|^2 \frac{|\langle \Psi_k^A || a_i^\dagger || \Psi_{k'}^{A-1} \rangle|^2}{(2J+1)(2T+1)}$$

- Sum of spectroscopic strength for an orbit  $i$

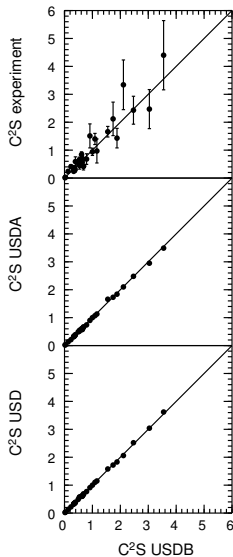
$$(2j_i + 1) = \sum_{k \in \mathcal{H}_{A+1}} \frac{2J_k + 1}{2J_0 + 1} C^2 S_k^+ + \sum_{k \in \mathcal{H}_{A-1}} C^2 S_k^-$$

- ESPE in reduced model space

$$(2j_i + 1) e_i^{cent} = (2j_i + 1) \epsilon = \sum_{k \in \mathcal{H}_{A+1}} \frac{2J_k + 1}{2J_0 + 1} C^2 S_k^+ E_k^+ + \sum_{k \in \mathcal{H}_{A-1}} C^2 S_k^- E_k^-$$

- Consistent treatment is required

# Comparison of experimental $C^2S$ in $sd$ shell to empirical interactions<sup>6</sup>



- Good agreement between all interactions and with experiment

# Exotic behavior

- Enhanced stability near the neutron dripline for oxygen isotopes
- New “shell closures” at  $N = 14$  and  $N = 16$
- Evaluate typical truncation procedures in isotopic chain
- Must understand effect of experimental limitations
- Truncate Baranger sum rule in reduced model space

$$\epsilon^{\text{trunc}} \equiv \frac{\sum_k^{\text{trunc}} (SF_k^+ E_k^+ + SF_k^- E_k^-)}{\sum_k^{\text{trunc}} (SF_k^+ + SF_k^-)}$$

- In terms of spectroscopic strength  $SF^\pm$
- In terms of excitation energy  $E_k^\pm$

# Exotic behavior

- Enhanced stability near the neutron dripline for oxygen isotopes
- New “shell closures” at  $N = 14$  and  $N = 16$
- Evaluate typical truncation procedures in isotopic chain
- **Must understand effect of experimental limitations**
- Truncate Baranger sum rule in reduced model space

$$\epsilon^{\text{trunc}} \equiv \frac{\sum_k^{\text{trunc}} (SF_k^+ E_k^+ + SF_k^- E_k^-)}{\sum_k^{\text{trunc}} (SF_k^+ + SF_k^-)}$$

- In terms of spectroscopic strength  $SF^\pm$
- In terms of excitation energy  $E_k^\pm$

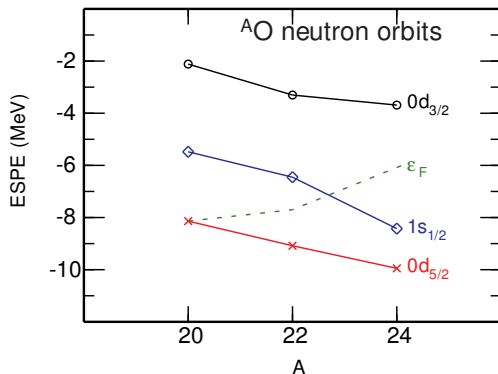
# Exotic behavior

- Enhanced stability near the neutron dripline for oxygen isotopes
- New “shell closures” at  $N = 14$  and  $N = 16$
- Evaluate typical truncation procedures in isotopic chain
- Must understand effect of experimental limitations
- **Truncate Baranger sum rule in reduced model space**

$$\epsilon^{\text{trunc}} \equiv \frac{\sum_k^{\text{trunc}} (SF_k^+ E_k^+ + SF_k^- E_k^-)}{\sum_k^{\text{trunc}} (SF_k^+ + SF_k^-)}$$

- In terms of spectroscopic strength  $SF^\pm$
- In terms of excitation energy  $E_k^\pm$

# Evolution of single particle shell structure

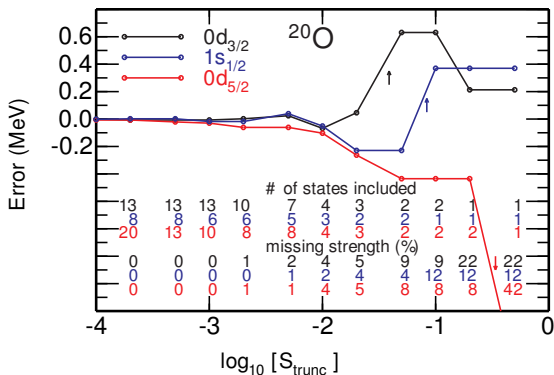


- Exotic oxygen isotopes
- $N = 16$  shell closure at  $A = 24$

Isotope	$E_{2_1^+}$ (th.)	$E_{2_1^+}$ (exp.)	$SF_0^{-/+}$	$\Delta e_F^{\text{ESPE}}$	Characterization
<sup>20</sup> O	1.87	1.67	0.58/0.34	0.00	Open-shell
<sup>22</sup> O	2.92	3.20	0.82/0.76	2.63	Closed-subshell
<sup>24</sup> O	4.78	4.72	0.89/0.92	4.74	Good closed-shell

# Truncation in spectroscopic strength

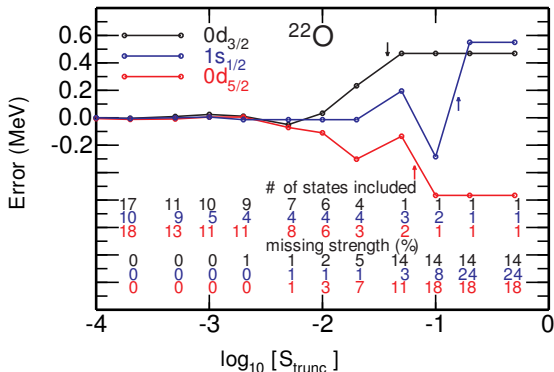
- A. Signoracci, T. Duguet, unpublished



- Open-shell  $\rightarrow$  both addition and removal channels required

# Truncation in spectroscopic strength

- A. Signoracci, T. Duguet, unpublished

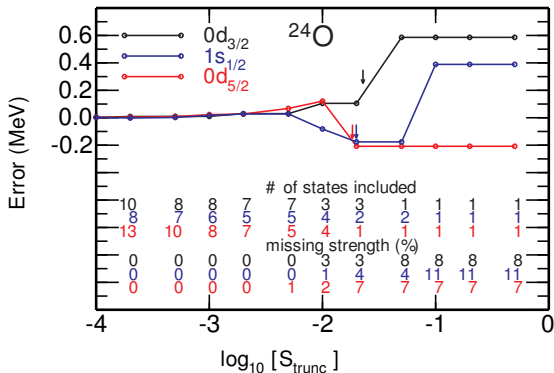


- Closed-subshell  $\rightarrow$  500 keV effect from lowest state of secondary channel
- Spin-orbit splitting affected by over 1 MeV by exclusion of **secondary channel**



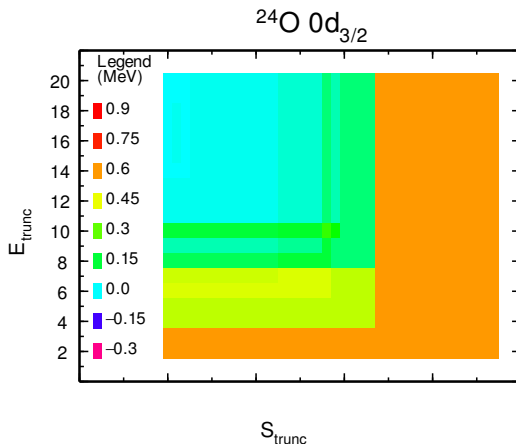
# Truncation in spectroscopic strength

- A. Signoracci, T. Duguet, unpublished



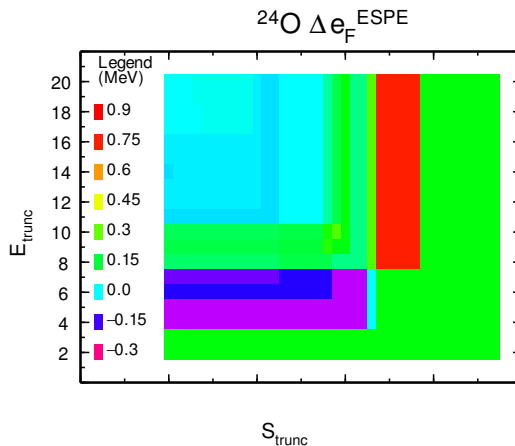
- Good closed-shell  $\rightarrow$  500 keV effect from secondary channel
- Need to include all  $SF \geq 0.01$  for desired precision

## Error based on truncation



- In all experiments, truncation in excitation energy and SF is necessary
- Effect on  $0d_{3/2}$  ESPE is 600 keV for  $E_{\text{trunc}} \leq 3$  or  $SF_{\text{trunc}} \geq 0.04$

# Error based on truncation



- Fermi gap can vary by 1 MeV for reasonable experimental conditions

# Outline

- 1 Introduction
- 2  $\beta$  decay
- 3 Electromagnetic transitions
- 4 Spectroscopic factors
- 5 Two-nucleon transfer/ other reaction model inputs

## Two-nucleon transfer

- Especially important decay mode near driplines
- Cannot reduce nuclear structure component to a simple number
- **Requires the use of two-body transition operators (TBTD)**
  - Formalism not presented here
  - Too complicated and less commonly utilized by practitioners
- **No examples in tutorial sessions**
  - Similar to procedure for one-nucleon transfer (spectroscopic factor)
  - Output in \*.tna file displays two-nucleon transfer amplitudes
- Typically used as input in reaction code calculation
  - Interference effects are important
  - Must be consistent in phase convention for wavefunctions

# Reaction model calculations

- **Common quantities utilized in reaction calculations**

- ① Spectroscopic factors (calculated with 'den' option of 'shell')
  - ② Two-nucleon amplitudes (calculated with 'den' option of 'shell')
  - ③ Single particle energies
    - Determine effective single particle energies by Baranger formula
    - Determine Skyrme, HO, or Woods-Saxon mean field SPE with 'dens' executable
  - ④ Single particle wavefunctions (calculated with 'dens' executable)
- Windows version includes executable for coupled-channels reaction code FRESKO
  - Many, many more possibilities
    - Learn by trial and error
    - Ask for more information relevant to your research