Introduction to NUSHELLX and transitions

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CEA/Saclay

Lecture 4, 24 April 2012

Outline

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Review

- Level schemes covered in Lecture III
  1. Calculate energies and wavefunctions with 'lpe' option of 'shell'
  2. NUSHELLX provides output in *.lpe,*.lpt, and *.eps files
- From the wavefunction, can determine many properties of interest
  1. β 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

$$e_p = 1.5e$$

$$e_n = 0.5e$$

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One-body transition densities

- One-body transition densities (OBTD)
  1. Provide the information to calculate matrix elements of one-body operators
  2. Compact, convenient form
  3. Different in J-scheme and m-scheme (only present J-scheme here)
  4. 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 λ

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

in a reduced model space with unique values of ℓ, j

- One-body transition densities between many-body states

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

- 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

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

- 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.)

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Outline

Introduction

- Primary method of decay for ground states of nuclei accessible with CI theory
  - $\beta^{\pm}$ decay converts a nucleus with (Z, A) to $(Z \mp 1, A)$
  - β^{+} 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

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

$x = 2$ for β^{+}

$x = 0$ for electron capture and β^{-}

Fermi and Gamow-Teller decay

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

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

- Fermi decay
  1. $\Delta J = 0$
  2. $\Delta T = 0$ (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
  1. $\Delta J = 0, 1$
  2. $\Delta T = 0, 1$ (isospin is good quantum number)

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

$\beta^{\pm}$ 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

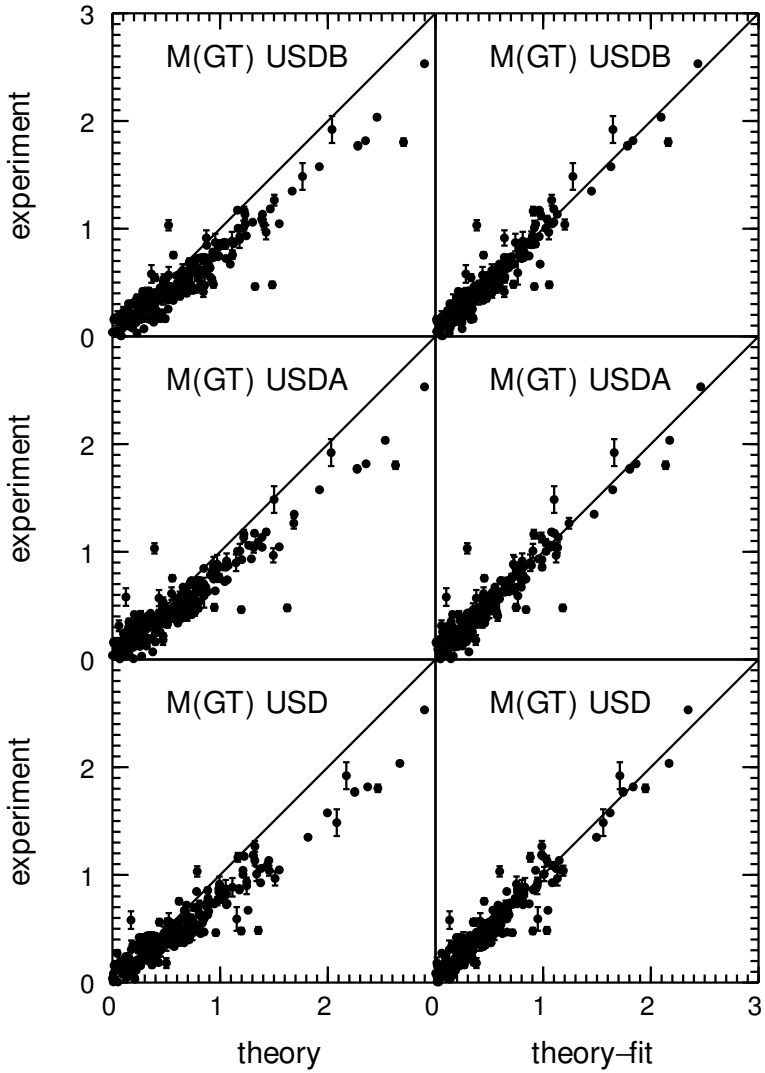
C = constant with the value 6170(4)

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[1]



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

[1] Courtesy of Alex Brown; from W.A. Richter et al., Phys. Rev. C **78**, 064302 (2008)

Outline

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 γ rays
- Sum of electric and magnetic multipole operators of tensor rank λ

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

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

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

- Free nucleon values:

$$e_p = 1 \quad g^\ell_p = 1 \quad g^s_p = 5.586$$
$$e_n = 0 \quad g^\ell_n = 0 \quad g^n_p = -3.826$$

Reduced transitions

- As described above

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

- Like the example for β 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

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

where

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

Reduced transitions

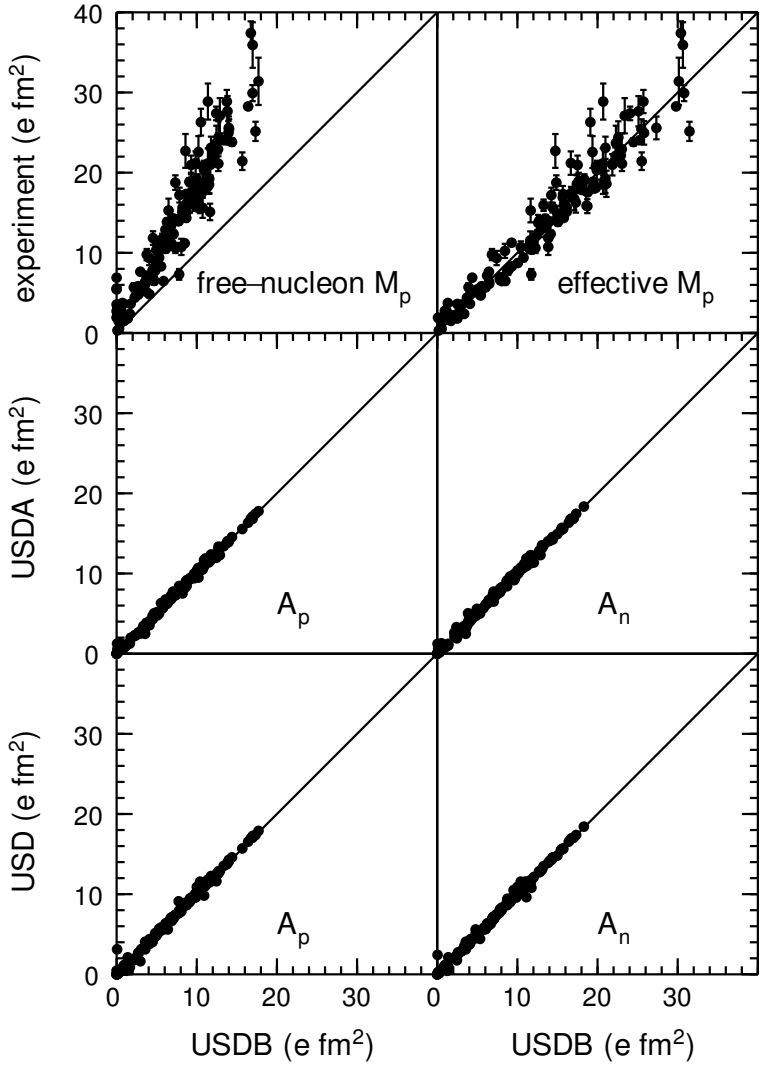
$$B(X\lambda; k' \to k) = \frac{|\langle \Psi_k || O(X\lambda) || \Psi_{k'} \rangle|^2}{2J_{k'} + 1} \equiv \frac{[M_{k,k'}(X\lambda)]^2}{2J_{k'} + 1}$$

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

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

- 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: $B(E2; \uparrow) \equiv B(E2; 0_1^+ \to 2_1^+)$
  - For γ decay: $B(E2; \downarrow) \equiv B(E2; 2_1^+ \to 0_1^+)$

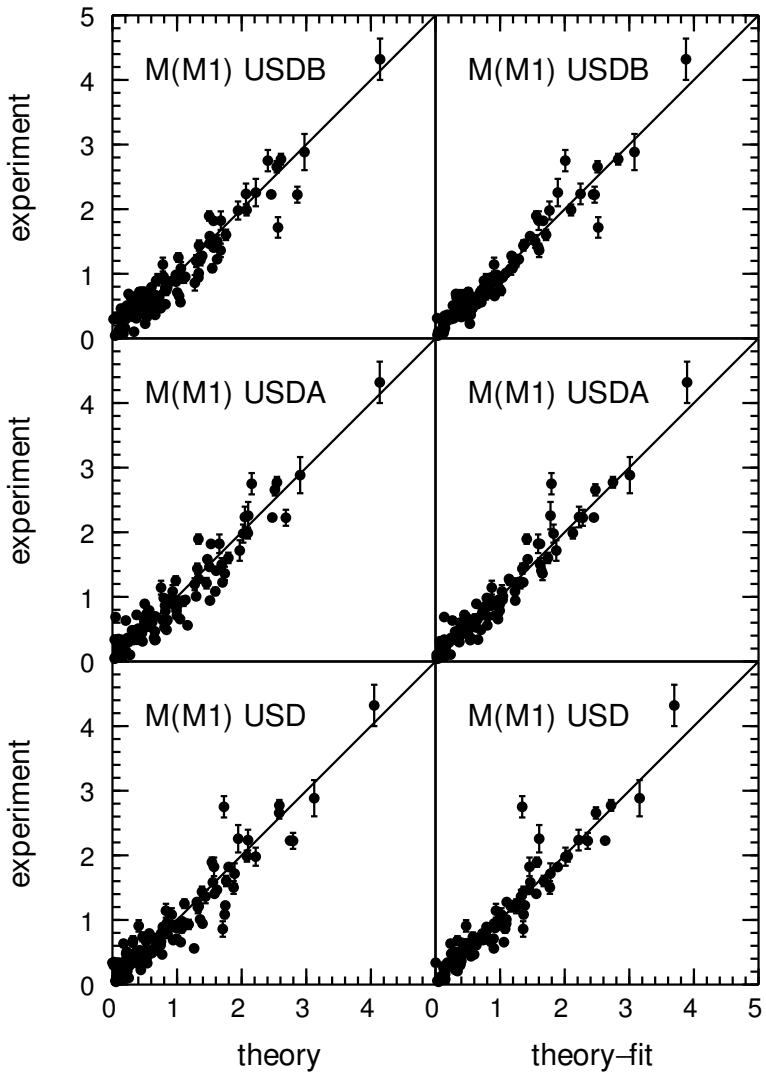
Comparison of experimental $M(E2)$ in *sd* shell to empirical interactions[2]



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

[2] 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[3]



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

[3] Courtesy of Alex Brown; from W.A. Richter et al., Phys. Rev. C **78**, 064302 (2008)

Outline

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[4]
- 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?[5]

[4] M. Baranger, Nucl. Phys. A **149**, 225 (1970)
[5] See T. Duguet and G. Hagen, Phys. Rev. C **85**, 034330 (2012)

Notation in NUSHELLX

- Written explicitly with dependence on isospin

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

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

- Sum of spectroscopic strength for an orbit i

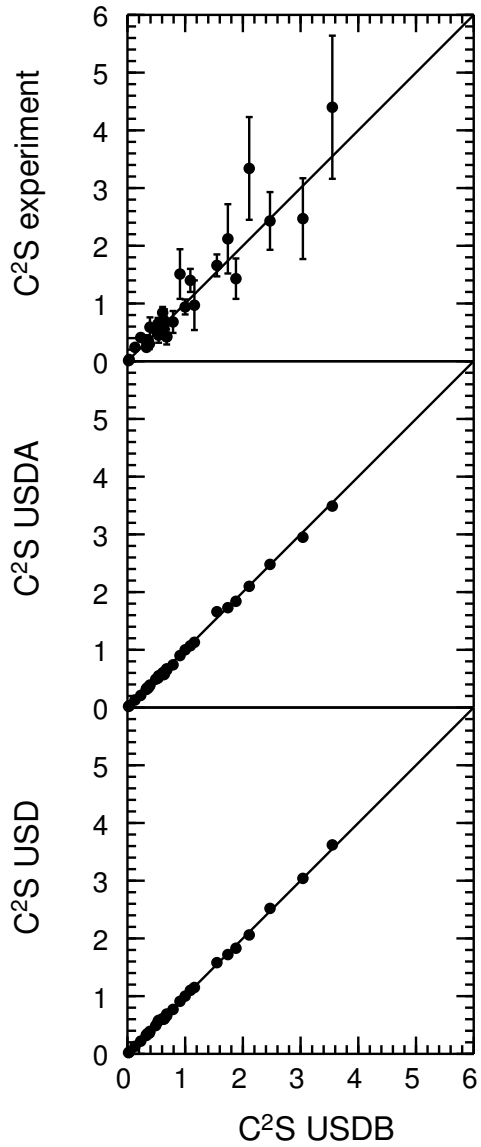
$$(2j_i+1) = \sum_{k\in\mathcal{H}_{A+1}} \frac{2J_k+1}{2J_0+1} C^2S_k^+ + \sum_{k\in\mathcal{H}_{A-1}} C^2S_k^-$$

- ESPE in reduced model space

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

- Consistent treatment is required

Comparison of experimental C^2S in *sd* shell to empirical interactions[6]



- 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 $E_k^{\pm}$

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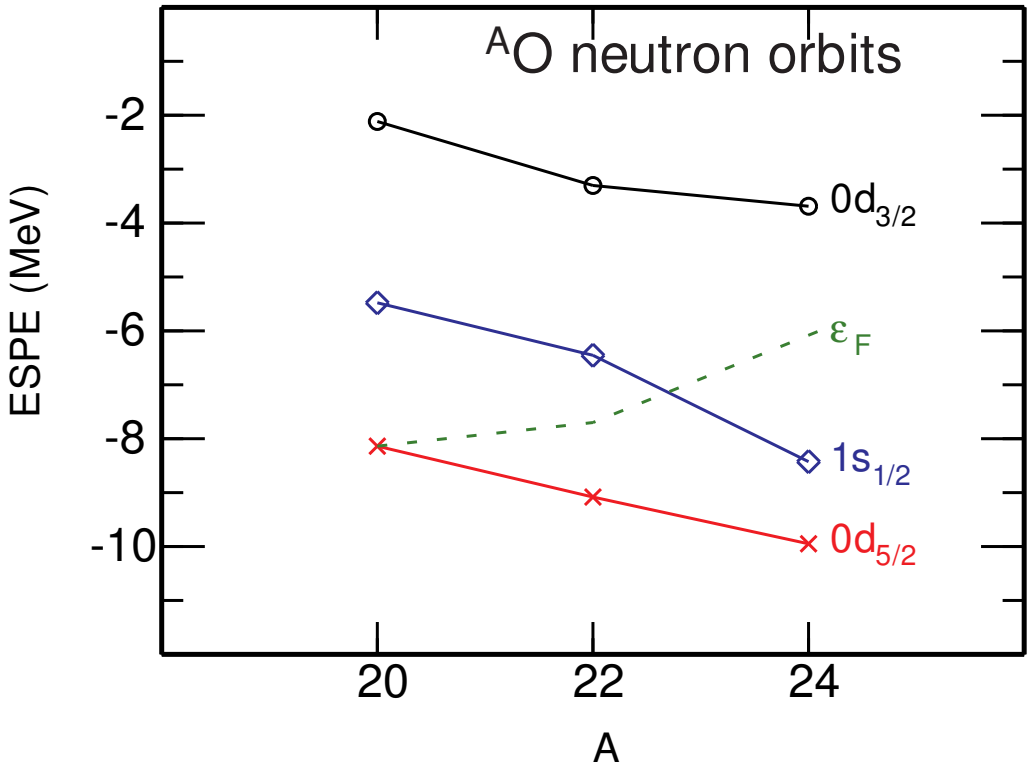
Evolution of single particle shell structure

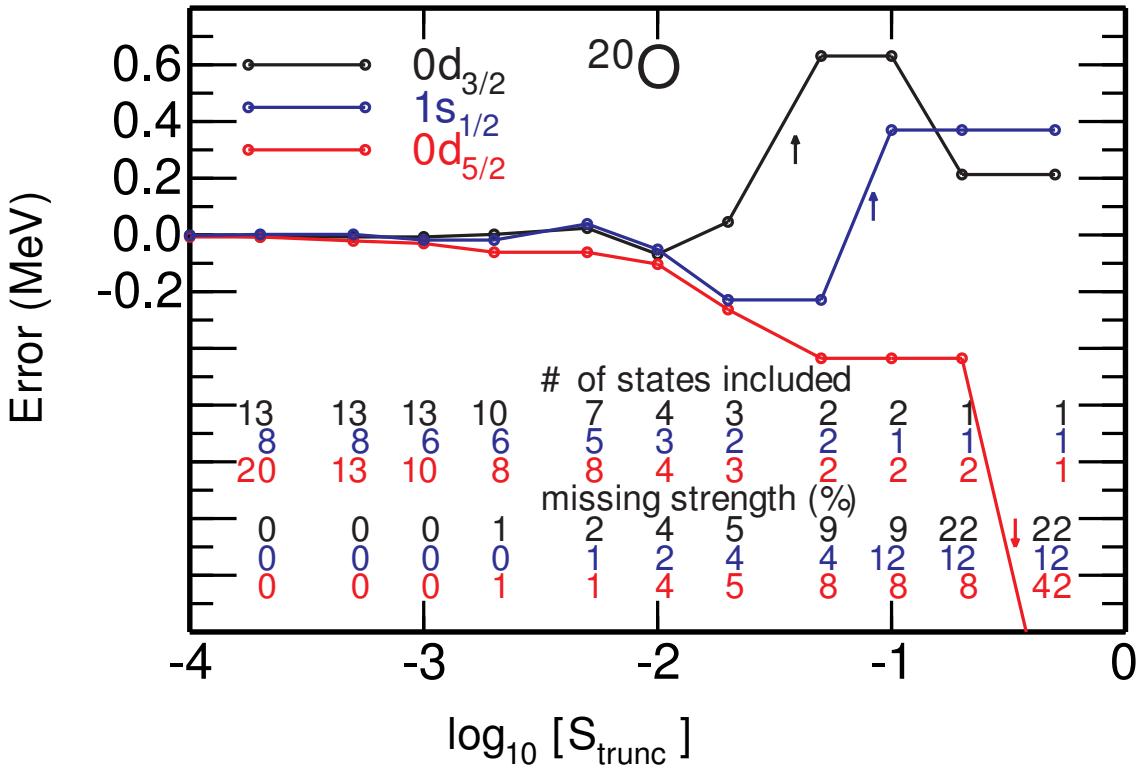


- Exotic oxygen isotopes
- $N = 16$ shell closure at $A = 24$

Isotope	$E_{2_1^+}$(th.)	$E_{2_1^+}$(exp.)	$SF_0^{-/+}$	$\Delta e_F^{\mathrm{ESPE}}$	Characterization
^{20}O	1.87	1.67	0.58/0.34	0.00	Open-shell
^{22}O	2.92	3.20	0.82/0.76	2.63	Closed-subshell
^{24}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

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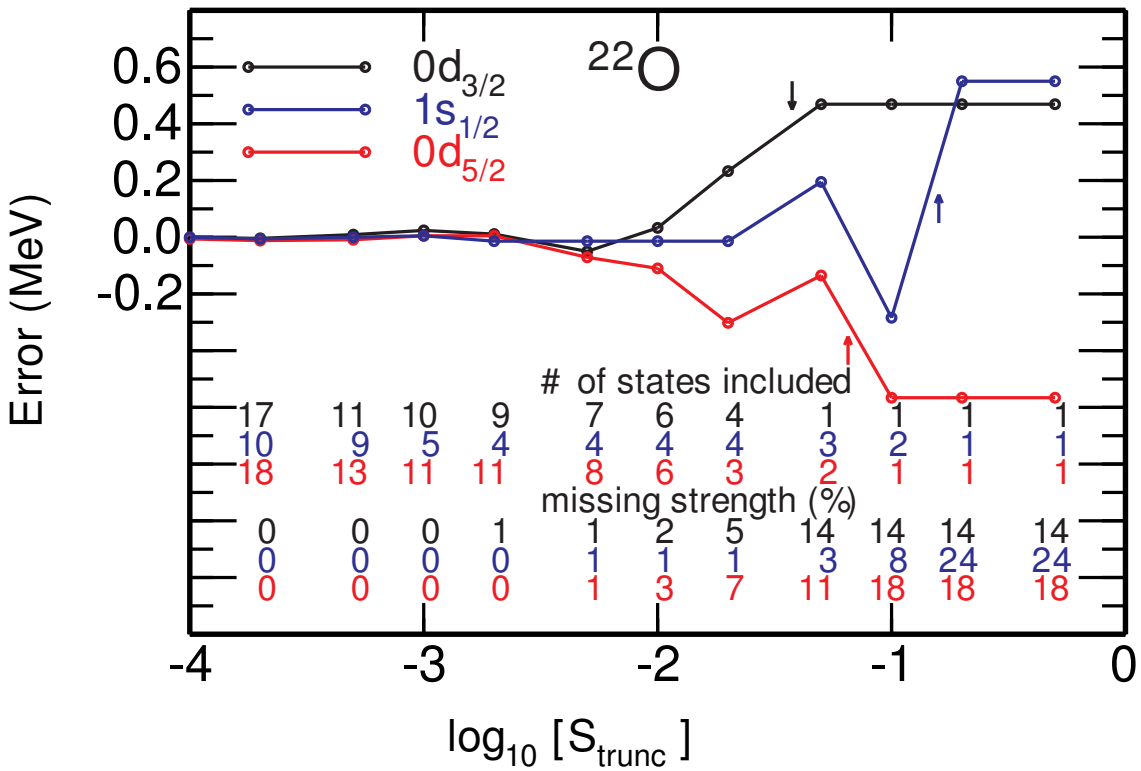

- Closed-subshell → 500 keV effect from lowest state of secondary channel
- Spin-orbit splitting affected by over 1 MeV by exclusion of secondary channel

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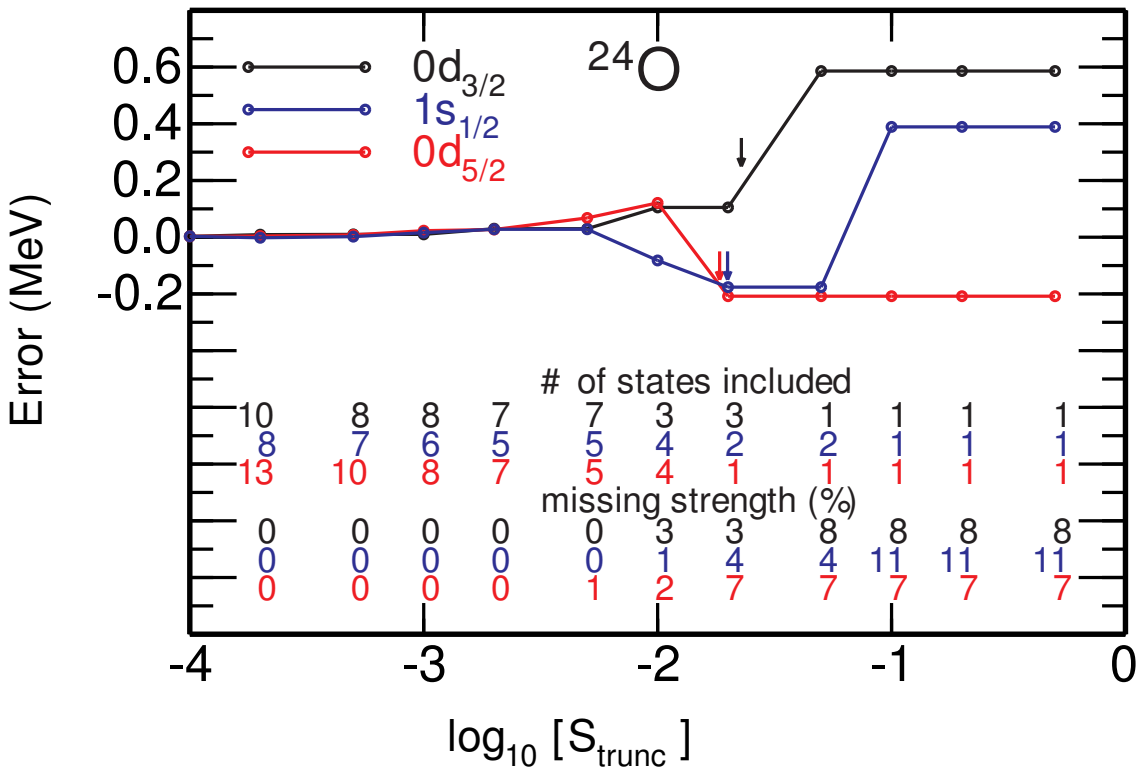
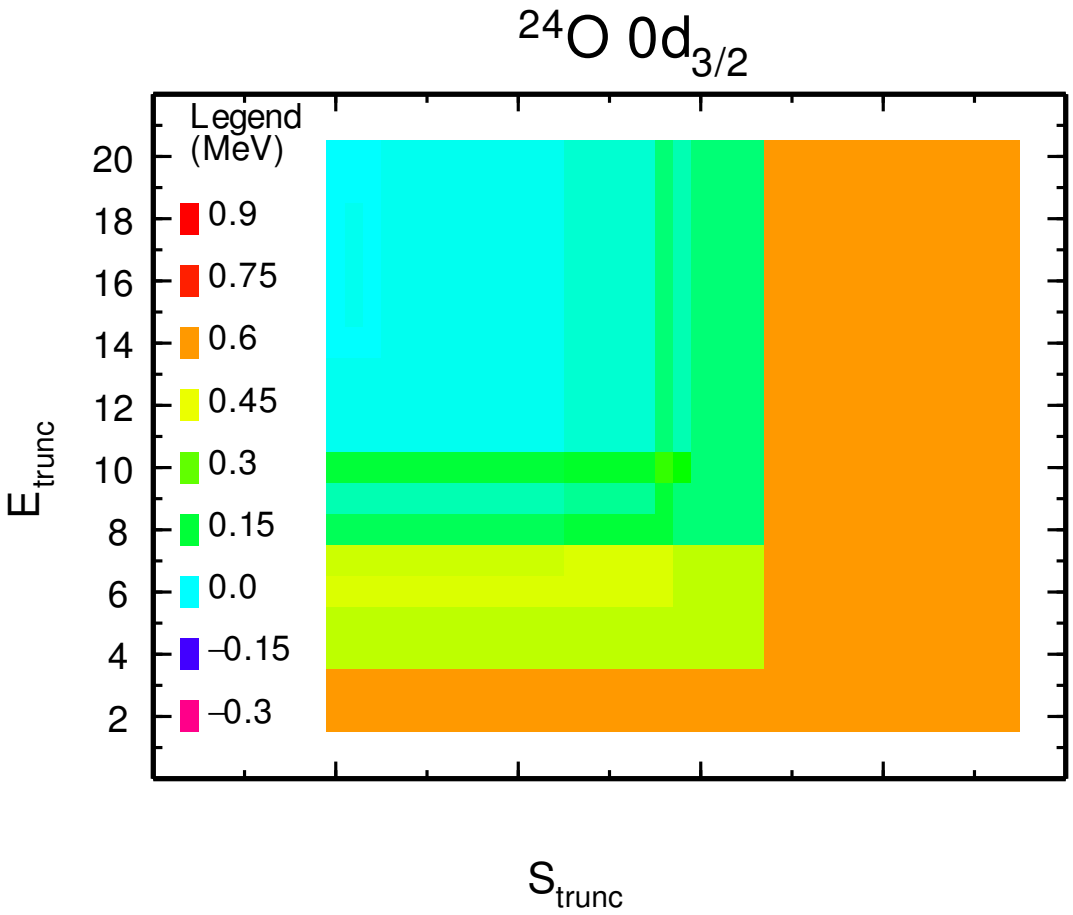


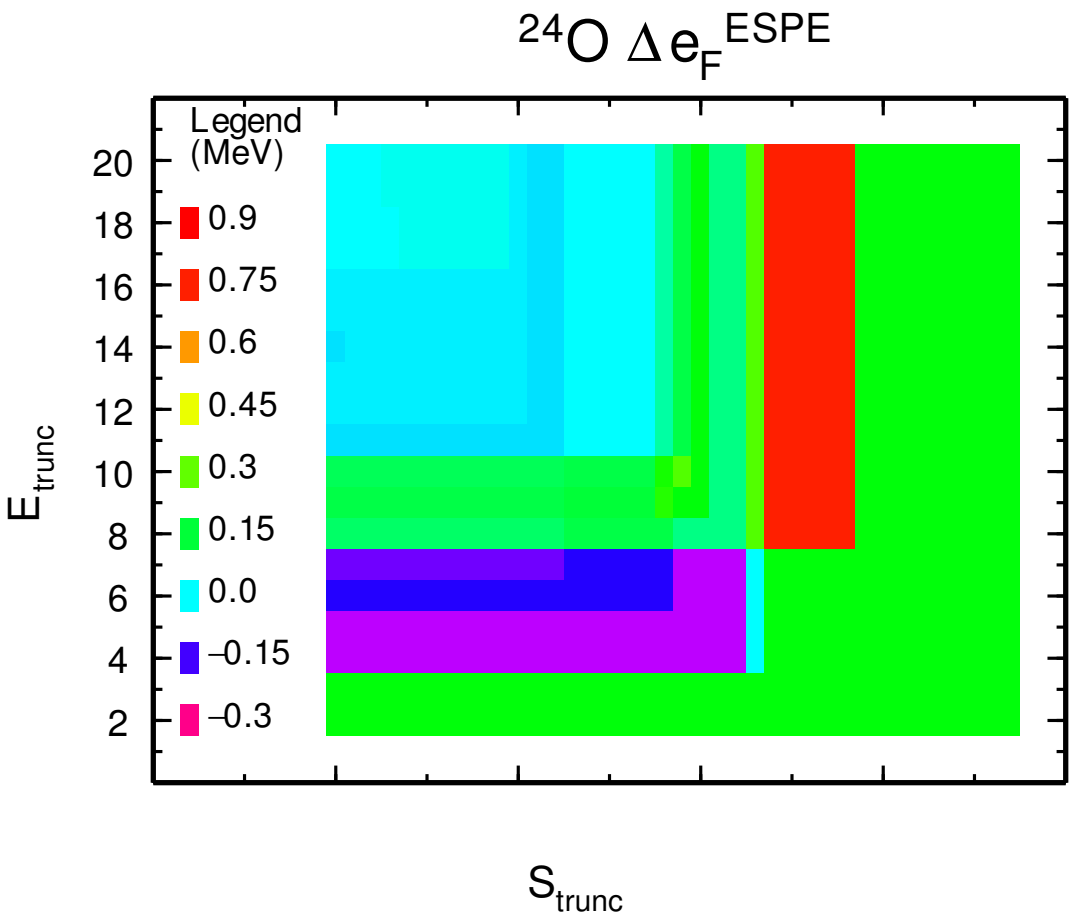
- Good closed-shell → 500 keV effect from secondary channel
- Need to include all SF ≥ 0.01 for desired precision

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

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 FRESCO
- Many, many more possibilities
  - Learn by trial and error
  - Ask for more information relevant to your research