

# Correlations and spectroscopic factors

**Angelo Signoracci** and Thomas Duguet

CEA/Saclay

07 February 2013

# Uncorrelated single particle shell structure

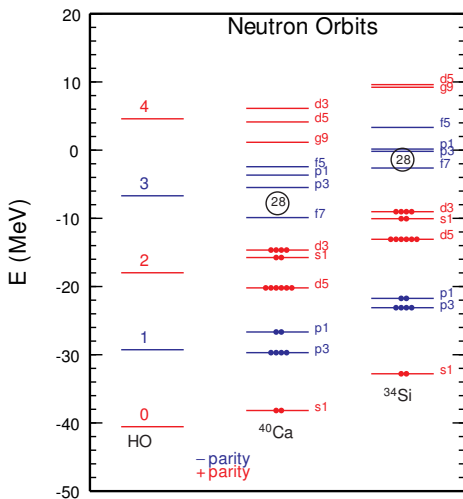
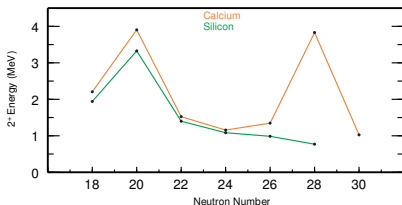
- Utilized to explain observations of correlated many-body observables
- E.g., exotic nuclei exhibit evolution of shell structure with  $N - Z$

- Many-body Schrödinger eq.

$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$$

- One-nucleon addition/removal

$$E_k^\pm = \pm(E_k^{A\pm 1} - E_0^A) \text{ and } \sigma_k^\pm$$



## Spectroscopic quantities

- Spectroscopic probability matrices

$$S_{\mu}^{+pq}(s) \equiv \langle \Psi_0^A(s) | a_p | \Psi_{\mu}^{A+1}(s) \rangle \langle \Psi_{\mu}^{A+1}(s) | a_q^{\dagger} | \Psi_0^A(s) \rangle$$

$$S_{\nu}^{-pq}(s) \equiv \langle \Psi_0^A(s) | a_q^{\dagger} | \Psi_{\nu}^{A-1}(s) \rangle \langle \Psi_{\nu}^{A-1}(s) | a_p | \Psi_0^A(s) \rangle$$

- Spectroscopic factors found from tracing spectroscopic probability matrices
  - Basis-independent, but not observable
- In reduced model space, recover typical “definitions”

$$SF_{\mu}^{+}(s) \equiv |\langle \Psi_{\mu}^{A+1}(s) | a_q^{\dagger} | \Psi_0^A(s) \rangle|^2$$

$$SF_{\nu}^{-}(s) \equiv |\langle \Psi_{\nu}^{A-1}(s) | a_p | \Psi_0^A(s) \rangle|^2$$

- Issues

- Variant results with identical, accurate many-body methods
- Experimental cross sections cannot be directly associated to spectroscopic values
- Practitioners are unwilling to relinquish single particle shell structure

- Advice

- Be consistent (in resolution scale, in many-body methods, etc.)
- Focus on relative values rather than absolute values
- Compare experimental observables (energy and cross section) to theoretical results
- Employ same theoretical method to produce non-observables ( $SF$  and ESPE)

## Spectroscopic quantities

- Spectroscopic probability matrices

$$S_{\mu}^{+pq}(s) \equiv \langle \Psi_0^A(s) | a_p | \Psi_{\mu}^{A+1}(s) \rangle \langle \Psi_{\mu}^{A+1}(s) | a_q^{\dagger} | \Psi_0^A(s) \rangle$$

$$S_{\nu}^{-pq}(s) \equiv \langle \Psi_0^A(s) | a_q^{\dagger} | \Psi_{\nu}^{A-1}(s) \rangle \langle \Psi_{\nu}^{A-1}(s) | a_p | \Psi_0^A(s) \rangle$$

- Spectroscopic factors found from tracing spectroscopic probability matrices
  - Basis-independent, but not observable
- In reduced model space, recover typical “definitions”

$$SF_{\mu}^{+}(s) \equiv |\langle \Psi_{\mu}^{A+1}(s) | a_q^{\dagger} | \Psi_0^A(s) \rangle|^2$$

$$SF_{\nu}^{-}(s) \equiv |\langle \Psi_{\nu}^{A-1}(s) | a_p | \Psi_0^A(s) \rangle|^2$$

- **Issues**
  - Variant results with identical, accurate many-body methods
  - Experimental cross sections cannot be directly associated to spectroscopic values
  - Practitioners are unwilling to relinquish single particle shell structure

- Advice

- Be consistent (in resolution scale, in many-body methods, etc.)
- Focus on relative values rather than absolute values
- Compare experimental observables (energy and cross section) to theoretical results
- Employ same theoretical method to produce non-observables ( $SF$  and ESPE)

## Spectroscopic quantities

- Spectroscopic probability matrices

$$S_{\mu}^{+pq}(s) \equiv \langle \Psi_0^A(s) | a_p | \Psi_{\mu}^{A+1}(s) \rangle \langle \Psi_{\mu}^{A+1}(s) | a_q^{\dagger} | \Psi_0^A(s) \rangle$$

$$S_{\nu}^{-pq}(s) \equiv \langle \Psi_0^A(s) | a_q^{\dagger} | \Psi_{\nu}^{A-1}(s) \rangle \langle \Psi_{\nu}^{A-1}(s) | a_p | \Psi_0^A(s) \rangle$$

- Spectroscopic factors found from tracing spectroscopic probability matrices
  - Basis-independent, but not observable
- In reduced model space, recover typical “definitions”

$$SF_{\mu}^{+}(s) \equiv |\langle \Psi_{\mu}^{A+1}(s) | a_q^{\dagger} | \Psi_0^A(s) \rangle|^2$$

$$SF_{\nu}^{-}(s) \equiv |\langle \Psi_{\nu}^{A-1}(s) | a_p | \Psi_0^A(s) \rangle|^2$$

- Issues
  - Variant results with identical, accurate many-body methods
  - Experimental cross sections cannot be directly associated to spectroscopic values
  - Practitioners are unwilling to relinquish single particle shell structure
- Advice
  - Be consistent (in resolution scale, in many-body methods, etc.)
  - Focus on relative values rather than absolute values
  - Compare experimental observables (energy and cross section) to theoretical results
  - Employ same theoretical method to produce non-observables ( $SF$  and ESPE)

# Effective single particle energies

## ● Requirements

- Define a single particle basis for the many-body problem of interest
- Solve by exclusively treating correlated many-body problem
- Independent of initial single particle basis
- Recover Hartree-Fock SPE in HF approximation

## ● (Relatively) Well-known prescription

- Method proposed by Baranger in Nucl. Phys. A **149**, 225 (1970)
- Can be determined by one solution to Schrödinger equation
- Requires summation over particle and hole states
- Basis-independent but not observable (depend on resolution scale  $s$ )

## ● Formalism

- Solution to eigenvalue problem  $h^{cent} \psi_p^{cent} = e_p^{cent} \psi_p^{cent}$ , where

$$h_{pq}^{cent} \equiv \sum_{\mu \in \mathcal{H}_{A+1}} S_{\mu}^{+pq} E_{\mu}^{+} + \sum_{\mu \in \mathcal{H}_{A-1}} S_{\mu}^{-pq} E_{\mu}^{-}$$

- In reduced model space, recover

$$e_p^{cent} \equiv \varepsilon = \sum_{\mu \in \mathcal{H}_{A+1}} SF_{\mu}^{+} E_{\mu}^{+} + \sum_{\mu \in \mathcal{H}_{A-1}} SF_{\mu}^{-} E_{\mu}^{-}$$

# Effective single particle energies

## ● Requirements

- Define a single particle basis for the many-body problem of interest
- Solve by exclusively treating correlated many-body problem
- Independent of initial single particle basis
- Recover Hartree-Fock SPE in HF approximation

## ● (Relatively) Well-known prescription

- Method proposed by Baranger in Nucl. Phys. A **149**, 225 (1970)
- Can be determined by one solution to Schrödinger equation
- Requires summation over particle and hole states
- Basis-independent but not observable (depend on resolution scale  $s$ )

## ● Formalism

- Solution to eigenvalue problem  $h^{cent} \psi_p^{cent} = e_p^{cent} \psi_p^{cent}$ , where

$$h_{pq}^{cent} \equiv \sum_{\mu \in \mathcal{H}_{A+1}} S_{\mu}^{+pq} E_{\mu}^{+} + \sum_{\mu \in \mathcal{H}_{A-1}} S_{\mu}^{-pq} E_{\mu}^{-}$$

- In reduced model space, recover

$$e_p^{cent} \equiv \varepsilon = \sum_{\mu \in \mathcal{H}_{A+1}} SF_{\mu}^{+} E_{\mu}^{+} + \sum_{\mu \in \mathcal{H}_{A-1}} SF_{\mu}^{-} E_{\mu}^{-}$$

# Effective single particle energies

- Requirements

- Define a single particle basis for the many-body problem of interest
- Solve by exclusively treating correlated many-body problem
- Independent of initial single particle basis
- Recover Hartree-Fock SPE in HF approximation

- (Relatively) Well-known prescription

- Method proposed by Baranger in Nucl. Phys. A **149**, 225 (1970)
- Can be determined by one solution to Schrödinger equation
- Requires summation over particle and hole states
- Basis-independent but not observable (depend on resolution scale  $s$ )

- **Formalism**

- Solution to eigenvalue problem  $h_p^{cent} \psi_p^{cent} = e_p^{cent} \psi_p^{cent}$ , where

$$h_{pq}^{cent} \equiv \sum_{\mu \in \mathcal{H}_{A+1}} S_{\mu}^{+pq} E_{\mu}^{+} + \sum_{\mu \in \mathcal{H}_{A-1}} S_{\mu}^{-pq} E_{\mu}^{-}$$

- In reduced model space, recover

$$e_p^{cent} \equiv \varepsilon = \sum_{\mu \in \mathcal{H}_{A+1}} SF_{\mu}^{+} E_{\mu}^{+} + \sum_{\mu \in \mathcal{H}_{A-1}} SF_{\mu}^{-} E_{\mu}^{-}$$



# Procedure

- Use configuration interaction technique to calculate  $sd$  shell nuclei
- Effective interactions determined semi-microscopically
  - ① Starting from underlying nucleon-nucleon potential (N3LO)
  - ② RG+MBPT to determine TBME in reduced model space
  - ③  $v_{lowk}$  cutoff  $\Lambda = 1.8, 1.9, \dots, 2.5 \text{ fm}^{-1}$  (8 interactions total)
  - ④ SPE taken from Skyrme Hartree Fock calculation with Skxtb interaction
- SPE from Skyrme Hartree-Fock theory are known to be unreliable
- Results depend on SPE, but primarily result in overall shift
- Could parameterize and fit to available data
- Also compared to new empirical USDB interaction
- For all even-even nuclei in the model space
  - Calculated lowest  $0^+, 2^+, 4^+$  states
  - Calculated all states accessible by one-nucleon addition or removal from g.s. ( $1/2^+, 3/2^+, 5/2^+$ )
  - Determined spectroscopic factors and ESPE

# Procedure

- Use configuration interaction technique to calculate  $sd$  shell nuclei
- Effective interactions determined semi-microscopically
  - ① Starting from underlying nucleon-nucleon potential (N3LO)
  - ② RG+MBPT to determine TBME in reduced model space
  - ③  $v_{lowk}$  cutoff  $\Lambda = 1.8, 1.9, \dots, 2.5 \text{ fm}^{-1}$  (8 interactions total)
  - ④ SPE taken from Skyrme Hartree Fock calculation with Skxtb interaction
- **SPE from Skyrme Hartree-Fock theory are known to be unreliable**
- Results depend on SPE, but primarily result in overall shift
- Could parameterize and fit to available data
- Also compared to new empirical USDB interaction
- For all even-even nuclei in the model space
  - Calculated lowest  $0^+, 2^+, 4^+$  states
  - Calculated all states accessible by one-nucleon addition or removal from g.s. ( $1/2^+, 3/2^+, 5/2^+$ )
  - Determined spectroscopic factors and ESPE

# Procedure

- Use configuration interaction technique to calculate  $sd$  shell nuclei
- Effective interactions determined semi-microscopically
  - ① Starting from underlying nucleon-nucleon potential (N3LO)
  - ② RG+MBPT to determine TBME in reduced model space
  - ③  $v_{lowk}$  cutoff  $\Lambda = 1.8, 1.9, \dots, 2.5 \text{ fm}^{-1}$  (8 interactions total)
  - ④ SPE taken from Skyrme Hartree Fock calculation with Skxtb interaction
- **SPE from Skyrme Hartree-Fock theory are known to be unreliable**
- Results depend on SPE, but primarily result in overall shift
- Could parameterize and fit to available data
- Also compared to new empirical USDB interaction
- For all even-even nuclei in the model space
  - Calculated lowest  $0^+, 2^+, 4^+$  states
  - Calculated all states accessible by one-nucleon addition or removal from g.s. ( $1/2^+, 3/2^+, 5/2^+$ )
  - Determined spectroscopic factors and ESPE

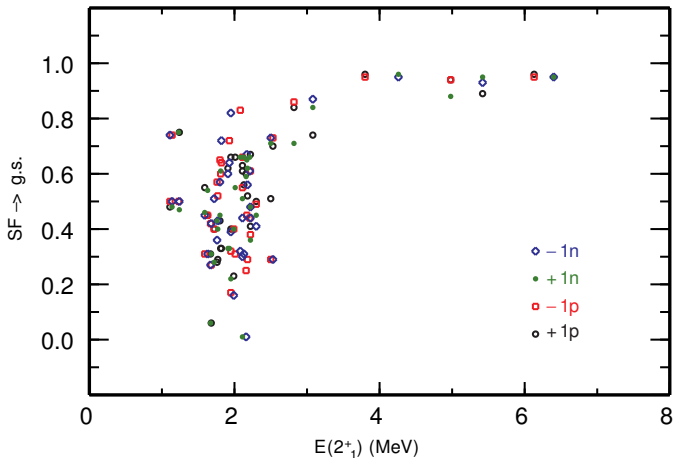
# Procedure

- Use configuration interaction technique to calculate  $sd$  shell nuclei
- Effective interactions determined semi-microscopically
  - ① Starting from underlying nucleon-nucleon potential (N3LO)
  - ② RG+MBPT to determine TBME in reduced model space
  - ③  $v_{lowk}$  cutoff  $\Lambda = 1.8, 1.9, \dots, 2.5 \text{ fm}^{-1}$  (8 interactions total)
  - ④ SPE taken from Skyrme Hartree Fock calculation with Skxtb interaction
- SPE from Skyrme Hartree-Fock theory are known to be unreliable
- Results depend on SPE, but primarily result in overall shift
- Could parameterize and fit to available data
- **Also compared to new empirical USDB interaction**
- For all even-even nuclei in the model space
  - Calculated lowest  $0^+, 2^+, 4^+$  states
  - Calculated all states accessible by one-nucleon addition or removal from g.s. ( $1/2^+, 3/2^+, 5/2^+$ )
  - Determined spectroscopic factors and ESPE

# Procedure

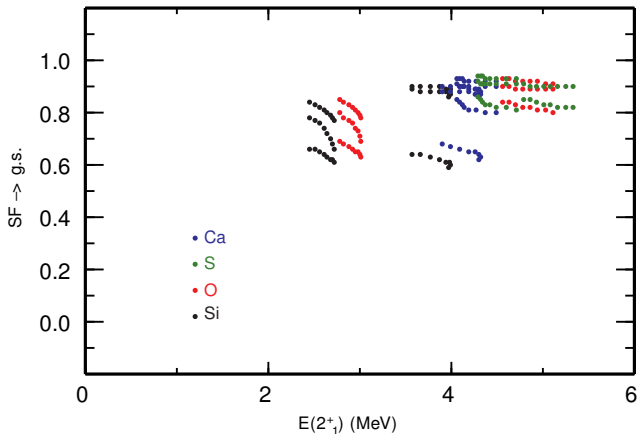
- Use configuration interaction technique to calculate  $sd$  shell nuclei
- Effective interactions determined semi-microscopically
  - ① Starting from underlying nucleon-nucleon potential (N3LO)
  - ② RG+MBPT to determine TBME in reduced model space
  - ③  $v_{lowk}$  cutoff  $\Lambda = 1.8, 1.9, \dots, 2.5 \text{ fm}^{-1}$  (8 interactions total)
  - ④ SPE taken from Skyrme Hartree Fock calculation with Skxtb interaction
- SPE from Skyrme Hartree-Fock theory are known to be unreliable
- Results depend on SPE, but primarily result in overall shift
- Could parameterize and fit to available data
- Also compared to new empirical USDB interaction
- **For all even-even nuclei in the model space**
  - Calculated lowest  $0^+, 2^+, 4^+$  states
  - Calculated all states accessible by one-nucleon addition or removal from g.s. ( $1/2^+, 3/2^+, 5/2^+$ )
  - Determined spectroscopic factors and ESPE

# Results with reference effective interaction $v_{ref}$ ( $\Lambda = 2.2 \text{ fm}^{-1}$ )



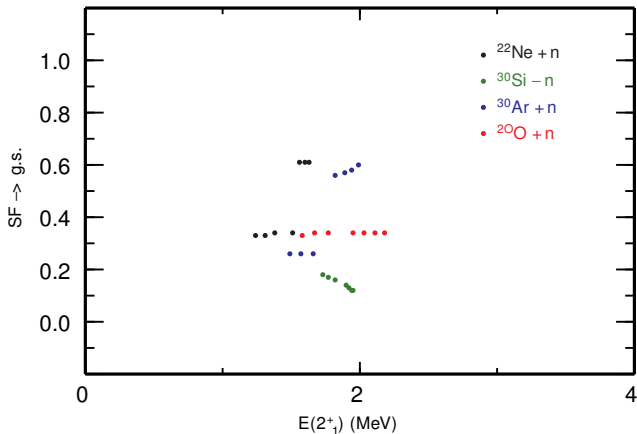
- 6-8 “doubly magic” nuclei
- Many states near 2 MeV with range of  $SF$

# Restriction to doubly magic nuclei



- Much fewer nuclei  $\rightarrow$  produce more points as a function of cutoff
- $SF$  at higher-energy are nearly constant with cutoff
- 20% effect for  $^{22}\text{O}$  and  $^{22}\text{Si}$

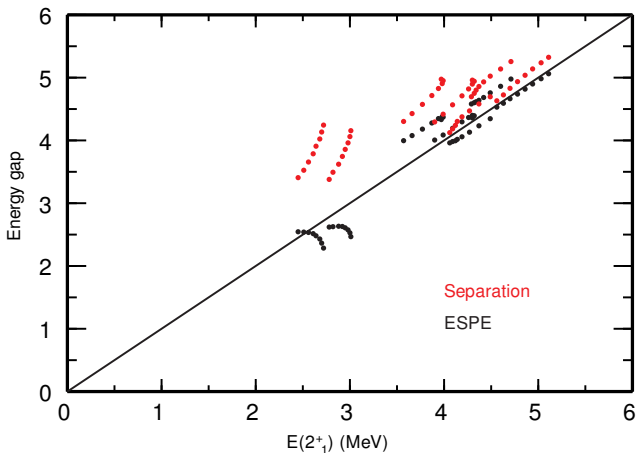
# Selected open-shell nuclei



- $E(2_1^+)$  decreases as cutoff increases
- $SF$  have inconsistent behavior as a function of cutoff
- Factor of 2 “jump” for  $^{22}\text{Ne}$ ,  $^{30}\text{Ar}$



# Energy gaps



- Separation energy gaps typically higher than  $E(2_1^+)$
- ESPE correlate better
- For  $^{22}\text{O}$  and  $^{22}\text{Si}$ , cutoff affects correlation

# Reconstructing ESPE

- In prior examples, summation over 200 states in removal and additional channel
- In each case, exhausted sum rule

$$1 = \sum_{\mu \in \mathcal{H}_{A+1}} SF_{\mu}^{+} + \sum_{\mu \in \mathcal{H}_{A-1}} SF_{\mu}^{-}$$

- Appropriate protocol
  - 1 Postulate consistent scheme
    - Maintain fixed  $H$  and  $s$  throughout
    - Consistent reaction/structure theory
  - 2 Validate theory against  $E_k^{\pm}(\text{exp})/\sigma_k^{\pm}(\text{exp})$
  - 3 Obtain  $S_k^{\pm}$  from structure calculation
- Truncate Baranger sum rule in reduced model space

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

- Evaluate typical truncation procedures in isotopic chain
  - Error on ESPE due to truncated strength?
  - Statistical uncertainty due to incomplete  $E_k^{\pm}(\text{exp})/\sigma_k^{\pm}(\text{exp})$ ?

# Reconstructing ESPE

- In prior examples, summation over 200 states in removal and additional channel
- In each case, exhausted sum rule

$$1 = \sum_{\mu \in \mathcal{H}_{A+1}} SF_{\mu}^{+} + \sum_{\mu \in \mathcal{H}_{A-1}} SF_{\mu}^{-}$$

- **Appropriate protocol**

- 1 Postulate consistent scheme
    - Maintain fixed  $H$  and  $s$  throughout
    - Consistent reaction/structure theory
  - 2 Validate theory against  $E_k^{\pm}(\text{exp})/\sigma_k^{\pm}(\text{exp})$
  - 3 Obtain  $S_k^{\pm}$  from structure calculation
- Truncate Baranger sum rule in reduced model space

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

- Evaluate typical truncation procedures in isotopic chain
  - Error on ESPE due to truncated strength?
  - Statistical uncertainty due to incomplete  $E_k^{\pm}(\text{exp})/\sigma_k^{\pm}(\text{exp})$ ?

# Reconstructing ESPE

- In prior examples, summation over 200 states in removal and additional channel
- In each case, exhausted sum rule

$$1 = \sum_{\mu \in \mathcal{H}_{A+1}} SF_{\mu}^{+} + \sum_{\mu \in \mathcal{H}_{A-1}} SF_{\mu}^{-}$$

- Appropriate protocol
  - 1 Postulate consistent scheme
    - Maintain fixed  $H$  and  $s$  throughout
    - Consistent reaction/structure theory
  - 2 Validate theory against  $E_k^{\pm}(\text{exp})/\sigma_k^{\pm}(\text{exp})$
  - 3 Obtain  $S_k^{\pm}$  from structure calculation
- Truncate Baranger sum rule in reduced model space

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

- Evaluate typical truncation procedures in isotopic chain
  - Error on ESPE due to truncated strength?
  - Statistical uncertainty due to incomplete  $E_k^{\pm}(\text{exp})/\sigma_k^{\pm}(\text{exp})$ ?

# Reconstructing ESPE

- In prior examples, summation over 200 states in removal and additional channel
- In each case, exhausted sum rule

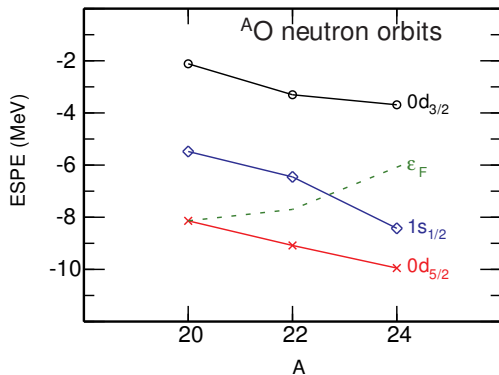
$$1 = \sum_{\mu \in \mathcal{H}_{A+1}} SF_{\mu}^{+} + \sum_{\mu \in \mathcal{H}_{A-1}} SF_{\mu}^{-}$$

- Appropriate protocol
  - 1 Postulate consistent scheme
    - Maintain fixed  $H$  and  $s$  throughout
    - Consistent reaction/structure theory
  - 2 Validate theory against  $E_k^{\pm}(\text{exp})/\sigma_k^{\pm}(\text{exp})$
  - 3 Obtain  $S_k^{\pm}$  from structure calculation
- Truncate Baranger sum rule in reduced model space

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

- Evaluate typical truncation procedures in isotopic chain
  - Error on ESPE due to truncated strength?
  - Statistical uncertainty due to incomplete  $E_k^{\pm}(\text{exp})/\sigma_k^{\pm}(\text{exp})$ ?

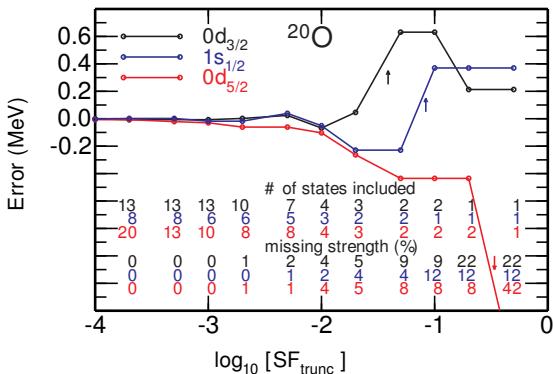
# Evolution of single particle shell structure



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

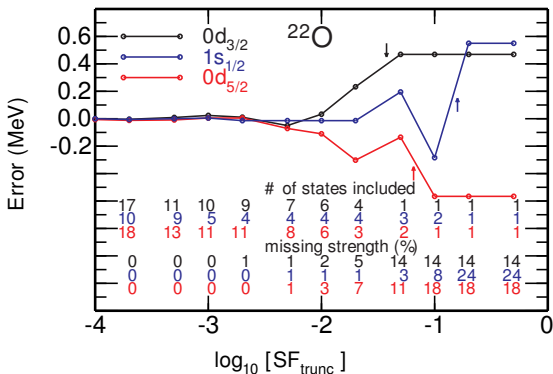
Isotope	$E_{2_1^+}$ (th.)	$E_{2_1^+}$ (exp.)	$SF_0^{-/+}$	$\Delta e_F^{\text{ESPE}}$	Characterization
<sup>20</sup> O	1.87	1.67	0.58/0.34	0.00	Open-shell
<sup>22</sup> O	2.92	3.20	0.82/0.76	2.63	Closed-subshell
<sup>24</sup> O	4.78	4.72	0.89/0.92	4.74	Good closed-shell

# Truncation in spectroscopic strength



- Open-shell  $\rightarrow$  both channels required

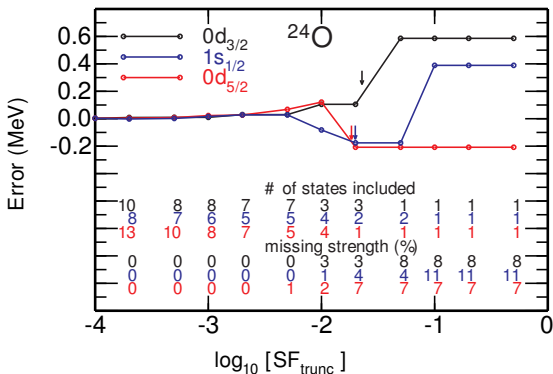
# Truncation in spectroscopic strength



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

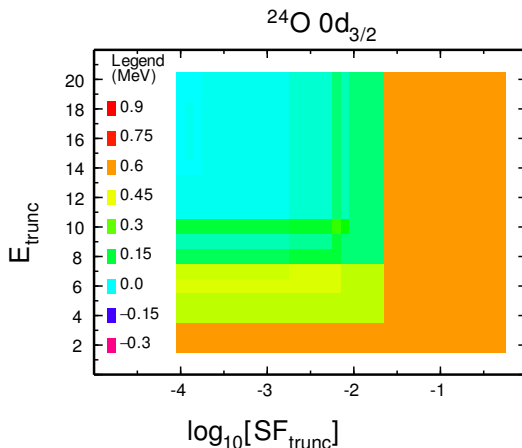


# Truncation in spectroscopic strength



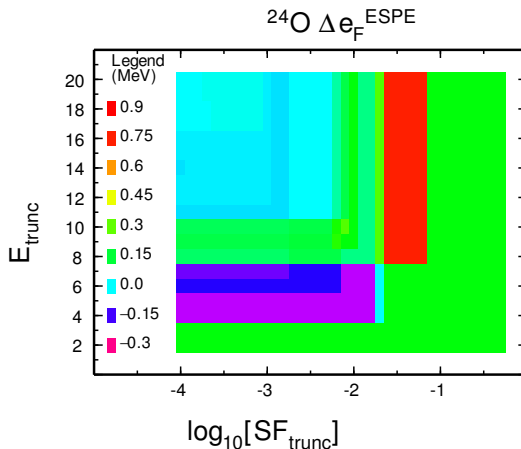
- Good closed-shell  $\rightarrow$  500 keV effect from secondary channel
- Need to include all  $SF \geq 0.01$  for desired precision

## Error based on truncation



- In all experiments, truncations in excitation energy and  $SF$  are 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

# Summary

- Microscopic interactions renormalized into nuclear medium
- Full-CI calculations performed in reduced model space
- $SF$  and ESPE are basis-independent but not observable
  - Depend on resolution scale  $s$
  - Consistent many-body methods are required for meaningful discussion
- Within one consistent scheme
  - Direct truncation of strength can result in 0.6 MeV error on ESPE
  - Even for good closed-shell nuclei
  - Error on Fermi gap and spin-orbit splitting  $> 1$  MeV
  - Even when reproducing (limited) data, large errors result
  - Must include primary and secondary channels to determine ESPE
- In order to discuss shell structure meaningfully
  - Employ a consistent scheme
  - Determine from theory (with a method that reproduces experimental observables)
  - Evaluate errors, e.g. statistically

# Summary

- Microscopic interactions renormalized into nuclear medium
- Full-CI calculations performed in reduced model space
- **$SF$  and ESPE are basis-independent but not observable**
  - Depend on resolution scale  $s$
  - Consistent many-body methods are required for meaningful discussion
- Within one consistent scheme
  - Direct truncation of strength can result in 0.6 MeV error on ESPE
  - Even for good closed-shell nuclei
  - Error on Fermi gap and spin-orbit splitting  $> 1$  MeV
  - Even when reproducing (limited) data, large errors result
  - Must include primary and secondary channels to determine ESPE
- In order to discuss shell structure meaningfully
  - Employ a consistent scheme
  - Determine from theory (with a method that reproduces experimental observables)
  - Evaluate errors, e.g. statistically

# Summary

- Microscopic interactions renormalized into nuclear medium
- Full-CI calculations performed in reduced model space
- $SF$  and ESPE are basis-independent but not observable
  - Depend on resolution scale  $s$
  - Consistent many-body methods are required for meaningful discussion
- **Within one consistent scheme**
  - Direct truncation of strength can result in 0.6 MeV error on ESPE
  - Even for good closed-shell nuclei
  - Error on Fermi gap and spin-orbit splitting  $> 1$  MeV
  - Even when reproducing (limited) data, large errors result
  - Must include primary and secondary channels to determine ESPE
- In order to discuss shell structure meaningfully
  - Employ a consistent scheme
  - Determine from theory (with a method that reproduces experimental observables)
  - Evaluate errors, e.g. statistically

# Summary

- Microscopic interactions renormalized into nuclear medium
- Full-CI calculations performed in reduced model space
- $SF$  and ESPE are basis-independent but not observable
  - Depend on resolution scale  $s$
  - Consistent many-body methods are required for meaningful discussion
- Within one consistent scheme
  - Direct truncation of strength can result in 0.6 MeV error on ESPE
  - Even for good closed-shell nuclei
  - Error on Fermi gap and spin-orbit splitting  $> 1$  MeV
  - Even when reproducing (limited) data, large errors result
  - Must include primary and secondary channels to determine ESPE
- In order to discuss shell structure meaningfully
  - Employ a consistent scheme
  - Determine from theory (with a method that reproduces experimental observables)
  - Evaluate errors, e.g. statistically