How shall we talk about the single-nucleon shell structure?

Unambiguous definition, non observability, reconstruction error and usefulness

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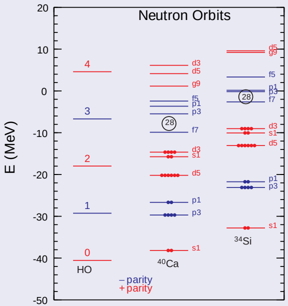
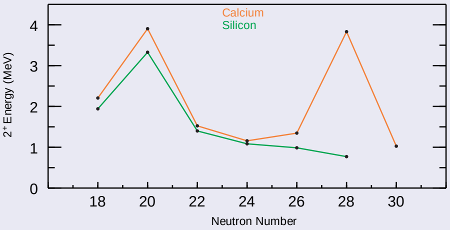
Context and questions

Interacting many-nucleon system

1. Uncorrelated single-nucleon shell structure $\{\epsilon^{A}_{nlj}\}$
   - Constitutes a pillar of our understanding of nuclear structure
   - Drives the physics of exotic nuclei via its evolution with N-Z





[Courtesy of A. Signoracci]

Context and questions

Nuclear many-body problem

1. Uncorrelated single-nucleon shell structure $\{\epsilon^{\mathrm{A}}_{nlj}\}$
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   - Drives the physics of exotic nuclei via its evolution with N-Z

2. Only the *correlated* A-body problem is uniquely defined

$$H|\Psi^{\mathrm{A}}_k\rangle = E^{\mathrm{A}}_k|\Psi^{\mathrm{A}}_k\rangle$$

such that one-nucleon addition and removal reactions give access to

$$E^{\pm}_k \equiv \pm\left(E^{\mathrm{A}\pm 1}_k - E^{\mathrm{A}}_0\right) \text{ and } \sigma^{\pm}_k$$

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such that one-nucleon pick-up and stripping reactions give access to

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In what sense shall we talk about $\{\epsilon^{\mathbf{A}}_{nlj}\}$?

↬ T. Duguet, G. Hagen, PRC85 (2012) 034330

Outline

1. Unambiguous definition
2. Non observability
3. Reconstruction error
4. Usefulness
5. Conclusions

Outline

Definition of effective single-particle energies (ESPEs)

Partitioning between "uncorrelated contribution" and "correlations"

$$\underbrace{\{E_k^{\pm}\,/\,|\Psi_0^{\mathrm{A}}\rangle\,;|\Psi_k^{\mathrm{A}\pm1}\rangle\}}_{\substack{A \\ \text{Outcome of Schr. equation}}} \equiv \underbrace{\{\epsilon_p\,/\,|\Phi_0^{\mathrm{A}}\rangle\,;|\Phi_p^{\mathrm{A}\pm1}\rangle\}}_{\substack{B \\ \text{Ind. particle contribution}}} + \underbrace{\{\Delta E_k^p\,/\,\delta|\Phi_k^p\rangle\}}_{\substack{C \\ \text{"The rest"}}}$$

B is usually

1. chosen = arbitrary partitioning
2. a priori = does not truly reflect A
3. as a zeroth-order approximation (HO, WS, HF...) = hoping to minimize C

Question of interest

Can $B = \{\epsilon_p\}$ be defined

1. exclusively from $A = \{E_k^{\pm}\,/\,|\Psi_0^{\mathrm{A}}\rangle\,;|\Psi_k^{\mathrm{A}\pm1}\rangle\}$?
2. independently of a zeroth-order approximation / single-particle basis used?
3. such that HF single-particle energies are recovered in HF approximation?

$\Rightarrow$ does an unambiguous definition of ESPEs deriving exclusively from A exist?

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Computing ESPEs (1)

Direct one-nucleon addition/removal on a $J^\pi = 0^+$ even-even ground state

1. One-nucleon separation energies

$$E^+_\mu \equiv E^{\mathrm{A}+1}_\mu - E^{\mathrm{A}}_0 \quad , \quad E^-_\nu \equiv E^{\mathrm{A}}_0 - E^{\mathrm{A}-1}_\nu$$

2. Spectroscopic amplitudes (U_μ, V_ν) represented in basis $\{a^\dagger_p\}$ $[p \equiv (n, l, j, m)]$

$$U^{p*}_\mu \equiv \langle \Psi^{\mathrm{A}+1}_\mu | a^\dagger_p | \Psi^{\mathrm{A}}_0 \rangle \quad , \quad V^{p*}_\nu \equiv \langle \Psi^{\text{A-1}}_\nu | a_p | \Psi^{\mathrm{A}}_0 \rangle$$

3. Spectroscopic "probability" matrix in basis $\{a^\dagger_p\}$

$$\begin{aligned} S^{+pq}_\mu &\equiv \langle \Psi^{\mathrm{A}}_0 | a_p | \Psi^{\mathrm{A}+1}_\mu \rangle \langle \Psi^{\mathrm{A}+1}_\mu | a^\dagger_q | \Psi^{\mathrm{A}}_0 \rangle \\ S^{-pq}_\nu &\equiv \langle \Psi^{\mathrm{A}}_0 | a^\dagger_q | \Psi^{\text{A-1}}_\nu \rangle \langle \Psi^{\text{A-1}}_\nu | a_p | \Psi^{\mathrm{A}}_0 \rangle \end{aligned}$$

4. Spectroscopic factors (basis independent)

$$SF^+_\mu \equiv \sum_{p \in \mathcal{H}_1} S^{+pp}_\mu \quad , \quad SF^-_\nu \equiv \sum_{p \in \mathcal{H}_1} S^{-pp}_\nu$$

provide the norm of one-nucleon overlap functions

Computing ESPEs (2)

Centroid matrix

1. Spectral-function $\mathbb{S}(\omega)$ (energy-dependent matrix)

$$\mathbb{S}_{pq}(\omega) \equiv \sum_{\mu \in \mathcal{H}_{A+1}} S_{\mu}^{+pq}\, \delta(\omega - E_{\mu}^{+}) + \sum_{\nu \in \mathcal{H}_{A-1}} S_{\nu}^{-pq}\, \delta(\omega - E_{\nu}^{-})$$

2. Moment of $\mathbb{S}(\omega)$ (energy-independent matrix)

$$\mathbb{M}_{pq}^{(n)} \equiv \int_{-\infty}^{+\infty} \omega^{n}\, \mathbb{S}_{pq}(\omega)\, d\omega$$

where $\mathbb{M}_{pq}^{(0)} = \delta_{pq}$ implies that $\mathbb{S}_{pp}(\omega)$ denotes a PDF for each p

3. Centroid matrix [M. Baranger, NPA149, 225 (1970)]

$$h_{pq}^{\text{cent}} \equiv \mathbb{M}_{pq}^{(1)} = \sum_{\mu \in \mathcal{H}_{A+1}} S_{\mu}^{+pq} E_{\mu}^{+} + \sum_{\nu \in \mathcal{H}_{A-1}} S_{\nu}^{-pq} E_{\nu}^{-}$$

which gathers information from both additional *and* removal channels

Computing ESPEs (3)

Effective single-particle energies

1. ESPEs $\equiv$ eigenvalues of the centroid matrix [M. Baranger, NPA149, 225 (1970)]

$$h^{\text{cent}}\,\psi_p^{\text{cent}} \quad = \quad e_p^{\text{cent}}\,\psi_p^{\text{cent}} \qquad [p \equiv (n,l,j,m)]$$

   - e_p^{cent} is the mean of the PDF $\mathbb{S}_{pp}(\omega)$ in basis $\{\psi_p^{\text{cent}}\}$
   - e_p^{cent} reduces to ϵ_p^{HF} in HF approximation

2. Basis-independent definition valid for any correlated system
   - Not valid to compute h_{pp}^{cent} in an arbitrarily chosen, e.g. HO, basis
   - Different from defining an unperturbed reference a priori

3. Two sets of connected but different wave functions and energies
   1. Overlap functions $\{U_\mu(\vec{r}\sigma\tau), V_\nu(\vec{r}\sigma\tau)\}$ decaying with $\{E_\mu^+, E_\nu^-\}$
   2. Centroid functions $\{\psi_p^{\text{cent}}(\vec{r}\sigma\tau)\}$ decaying with $\{e_p^{\text{cent}}\}$

Computing ESPEs (4)

Sum rule and correlations

1. Identity for n^{th} moment of $\mathbb{S}(\omega)$

$$\mathbb{M}^{(n)}_{pq} \quad = \quad \langle \Psi^{\mathrm{A}}_0 | \{ \overbrace{[\ldots[[a_p, H], H], \ldots]}^{n\,\text{commutators}}, a^{\dagger}_q \} | \Psi^{\mathrm{A}}_0 \rangle$$

2. Applied to $n = 1$ [M. Baranger, NPA149, 225 (1970)]

$$h^{\text{cent}}_{pq} \quad = \quad T_{pq} + \sum_{rs} \bar{V}^{2\mathrm{N}}_{prqs}\, \rho^{[1]}_{sr} + \frac{1}{4} \sum_{rstv} \bar{V}^{3\mathrm{N}}_{prtqsv}\, \rho^{[2]}_{svrt} = h^{\infty}_{pq}$$

   - Accessing ESPEs only require to compute $|\Psi^{\mathrm{A}}_0\rangle$
   - $e^{\text{cent}}_p - \epsilon^{\mathrm{HF}}_p \neq 0$ due to correlations in $\rho^{[k]}$
   - $h^{\infty} \equiv T+$ energy-independent part of $\Sigma(\omega)$ in Dyson-SCGF

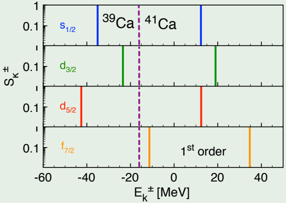
3. Centroids screen out most of the correlations [M. Dufour, A. Zuker, PRC54, 1641 (1996)]
   - Only monopole part of interactions $V^{\text{mon}} \equiv \sum_J (2J+1)\, V^J$ involved
   - Higher multipoles responsible for genuine correlation effects

Why separation energies cannot be confused with ESPEs?

Spectral-strength distribution

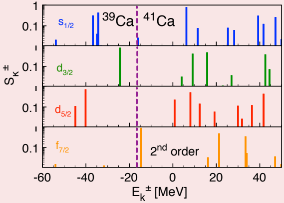
$$\mathcal{S}(\omega) \equiv \mathrm{Tr}_{\mathcal{H}_1}\left[\mathbb{S}(\omega)\right] = \sum_{\mu \in \mathcal{H}_{A+1}} SF_{\mu}^{+}\, \delta(\omega - E_{\mu}^{+}) + \sum_{\nu \in \mathcal{H}_{A-1}} SF_{\nu}^{-}\, \delta(\omega - E_{\nu}^{-})$$

Uncorrelated system



1. $SF_{\mu}^{\pm} = 0$ or 1
2. $\mathrm{Card}\{SF_{\mu}^{\pm} \neq 0\} = \dim_{\mathcal{H}_1}$

Correlated system



1. $0 < SF_{\mu}^{\pm} < 1$
2. $\mathrm{Card}\{SF_{\mu}^{\pm} \neq 0\} > \dim_{\mathcal{H}_1}$

- Direct addition and removal populate more states than $\dim_{\mathcal{H}_1}$
- $(E_{\mu}^{\pm}, SF_{\mu}^{\pm})$ spectrum does not possess features of single-particle spectrum

From an uncorrelated to a correlated system

EOM-CCSD calculations in Gamow-Hartree-Fock basis

1. $H = T + V^{2N}$ = Chiral N^{3}LO with Λ_χ =500 MeV
2. $H(\Lambda) = T + V^{2N}(\Lambda)$ with $\Lambda \in [2.0; 3.0]$ fm^{-1} ($V^{3N\cdots}(\Lambda) = 0 \Rightarrow U(\Lambda)\,U^\dagger(\Lambda) \neq 1$)
3. HO single-particle basis ($n_{\max} = 12$; $\hbar\omega$ =16 MeV) + 30 WS $2s_{1/2}$ orbitals

Probing the effect of correlations

1. Normal ordering of H with respect to $|\Phi^{\mathrm{HF}}\rangle$ in HF single-particle basis

$$H = E^{\mathrm{HF}} + \sum_p \epsilon_p^{\mathrm{HF}} : b_p^\dagger b_p : + \frac{1}{4} \sum_{pqrs} \bar{V}^{2N}_{pqrs} : b_p^\dagger b_q^\dagger b_s b_r : \equiv h^{\mathrm{HF}} + V_{\mathrm{res}}$$

$$\epsilon_p^{\mathrm{HF}} = T_{pp} + \sum_{q=1}^{A} \bar{V}^{2N}_{pqpq}$$

2. Define $V_{\mathrm{res}}(\lambda) \equiv \lambda\, V_{\mathrm{res}}$ such that $H(0) = h^{\mathrm{HF}}$ and $H(1) = H$
3. Solve EOM-CCSD repeatedly for $\lambda \in [0, 1]$

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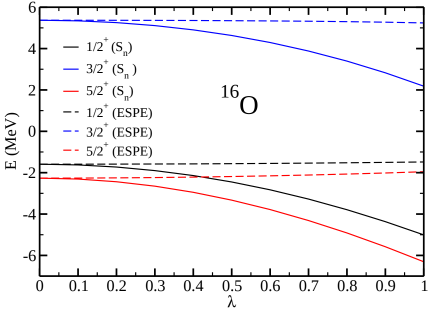


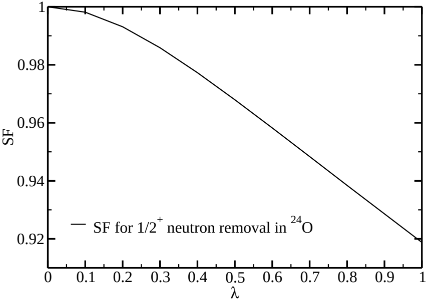
Doubly-magic ^{16}O

- Neutron $E^{+}_{\mu}(\lambda)$ versus $e^{\text{cent}}_{p}(\lambda)$
- $\Lambda = 2.4\,\text{fm}^{-1}$

Switching on correlations

1. Uncorrelated limit: $e^{\text{cent}}_{p}(0) = E^{+}_{\mu}(0) = \epsilon^{\text{HF}}_{p}$ (Koopman's theorem)
2. Strongly correlated system as $E^{+}_{\mu}(1) - e^{\text{cent}}_{p}(1) \approx -3\,\text{MeV}$
3. Centroid energies almost untouched by correlations as $\partial_{\lambda}\, e^{\text{cent}}_{p}(\lambda) \approx 0$
4. Both would be significantly more affected in open-shell nuclei

From an uncorrelated to a correlated system



$J^\pi = 1/2^+$ neutron removal in ^{24}O

1. $SF^-_{1/2+}(\lambda)$
2. $E^-_{1/2+}(\lambda)$ versus $e^{\text{cent}}_{2s_{1/2}}(\lambda)$

Switching on correlations in doubly-magic ^{24}O

1. Based on $SF^-_{1/2+}(1)$ the state has a strong single-particle character
2. Energy shift is however significant $E^-_{1/2+}(1) - e^{\text{cent}}_{2s_{1/2}}(1) \approx -1.7\,\text{MeV}$
   - Small fragmented strength rejected to rather high missing energies
3. SM works with effective closed core and limited explicit dynamics
   - e_p^{core} coming out of fit (e.g. USDB) effectively account for $e_p^{\text{cent. val. space}}$

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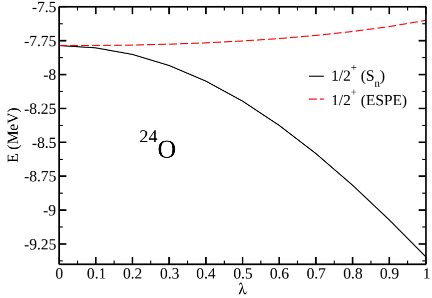

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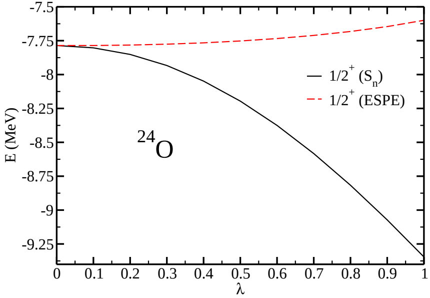

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Outline

Observable and non observable

Low-energy nuclear many-body problem

1. A-body problem defined within a consistent EFT at a given order in $(Q/\Lambda_\chi)^\nu$

$$\left.\begin{array}{rl} \text{Hamiltonian} & H \equiv \sum_\nu H^{(\nu)} \\[2ex] \text{Other operator} & O \equiv \sum_\nu O^{(\nu)} \end{array}\right\} \Longrightarrow \left\{\begin{array}{l} H|\Psi_k^{\mathrm{A}}\rangle = E_k^{\mathrm{A}}|\Psi_k^{\mathrm{A}}\rangle \\[2ex] O_k^{\mathrm{A}} = \langle\Psi_k^{\mathrm{A}}|O|\Psi_k^{\mathrm{A}}\rangle \end{array}\right.$$

2. Unitary transformation $U(\Lambda)$ over Fock space
   1. $H(\Lambda) \equiv U(\Lambda)\, H\, U^\dagger(\Lambda)$ leads to $\left\{\begin{array}{l} H(\Lambda)|\Psi_k^{\mathrm{A}}(\Lambda)\rangle = E_k^{\mathrm{A}}|\Psi_k^{\mathrm{A}}(\Lambda)\rangle \\[2ex] |\Psi_k^{\mathrm{A}}(\Lambda)\rangle \equiv U(\Lambda)\,|\Psi_k^{\mathrm{A}}\rangle \end{array}\right.$
   2. Observable $O(\Lambda) \equiv U(\Lambda)\, O\, U^\dagger(\Lambda)$ leads to $\langle\Psi_k^{\mathrm{A}}(\Lambda)|O(\Lambda)|\Psi_k^{\mathrm{A}}(\Lambda)\rangle = O_k^{\mathrm{A}}$
   3. Not transforming operator O defines a non-observable quantity as

$$\partial_\Lambda \langle\Psi_k^{\mathrm{A}}(\Lambda)|O|\Psi_k^{\mathrm{A}}(\Lambda)\rangle \neq 0$$

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Observable and non observable

Spectroscopic amplitudes are not observable [B. K. Jennings (2011), arXiv:1102.3721]

1. One-nucleon overlap functions are defined for any Λ through

$$U_k^p(\Lambda) \equiv \langle \Psi_k^{A+1}(\Lambda) | a_p^\dagger | \Psi_0^A(\Lambda) \rangle^* \quad ; \quad V_k^p(\Lambda) \equiv \langle \Psi_k^{A\text{-}1}(\Lambda) | a_p | \Psi_0^A(\Lambda) \rangle^*$$

as using $U(\Lambda)\, a_p^\dagger\, U^\dagger(\Lambda) = \sum_q u_q^p a_q^\dagger + \sum_{qrs} u_{qrs}^p a_q^\dagger a_r^\dagger a_s + \ldots$ would kill the purpose

2. Spectroscopic amplitudes vary under $U(\Lambda)$ and are not observable

Scale dependence of ESPEs

Similarity renormalization group transformation $H(s) \equiv U(s) H U^\dagger(s)$

1. RG flow for operators and states

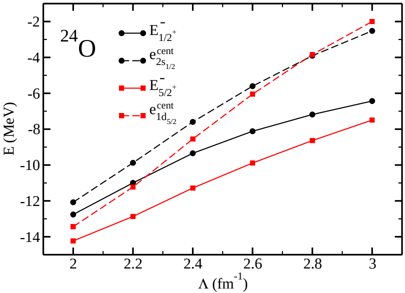
$$\frac{d}{ds} O(s) \equiv [\eta(s), O(s)] \qquad \text{where} \quad \eta(s) \equiv \frac{dU(s)}{ds} U^\dagger(s) = -\eta^\dagger(s)$$

$$\frac{d}{ds} |\Psi^{\mathrm{A}}_{\mu}(s)\rangle \equiv \eta(s) |\Psi^{\mathrm{A}}_{\mu}(s)\rangle$$

2. RG flow for the quantities of interest

$$\begin{aligned}
\frac{d}{ds} S^{-pq}_{\nu}(s) &= -\langle \Psi^{\mathrm{A}}_0(s) | [\eta(s), a^\dagger_p] | \Psi^{\mathrm{A\text{-}1}}_{\nu}(s)\rangle \langle \Psi^{\mathrm{A\text{-}1}}_{\nu}(s) | a_q | \Psi^{\mathrm{A}}_0(s)\rangle \\
&\quad -\langle \Psi^{\mathrm{A}}_0(s) | a^\dagger_p | \Psi^{\mathrm{A\text{-}1}}_{\nu}(s)\rangle \langle \Psi^{\mathrm{A\text{-}1}}_{\nu}(s) | [\eta(s), a_q] | \Psi^{\mathrm{A}}_0(s)\rangle \neq 0 \\
\frac{d}{ds} E^{-}_{\nu}(s) &= 0 \\
\frac{d}{ds} \mathbb{M}^{(0)}_{pq}(s) &= 0 \\
\frac{d}{ds} \mathbb{M}^{(1)}_{pq}(s) &= -\langle \Psi^{\mathrm{A}}_0(s) | \{[[\eta(s), a_p], H(s)], a^\dagger_q\} | \Psi^{\mathrm{A}}_0(s)\rangle \\
&\quad -\langle \Psi^{\mathrm{A}}_0(s) | \{[a_p, H(s)], [\eta(s), a^\dagger_q]\} | \Psi^{\mathrm{A}}_0(s)\rangle \neq 0
\end{aligned}$$

Scale dependence of ESPEs in CC calculations



One-neutron removal in ^{24}O

- E_ν^- and e_p^{cent} versus Λ
- $\Lambda \in [2.0; 3.0]$ fm^{-1}

Non-absoluteness of ESPEs

1. Scale dependence of E_ν^- from omitted induced forces and clusters
2. Intrinsic scale dependence of $e_p^{cent} \approx 6$ MeV for $\Lambda \in [2.0, 3.0]$ fm^{-1}
   - Not identical for all shells
3. Clean demonstration demands unitarily equivalent calculations
   - Requires to track (at least) 3N forces
   - NCSM and CCSD(T) calculations [T. D., K. Hebeler, G. Hagen, D. Furnstahl]

Non-absoluteness of ESPEs

Spectroscopic amplitudes are not observable [B. K. Jennings (2011), arXiv:1102.3721]

ESPEs (wave-functions, SFs, correlations...) are not observable

$$\underbrace{A}_{\{E_k^\pm;\sigma_k^\pm\}\text{ invariant under } U(\Lambda)}^{\text{Many-body observable}} \equiv \underbrace{B}_{\{e_p^{\text{cent}};\sigma_p^{\text{s.p.}}\}\text{ varies under } U(\Lambda)}^{\text{Single-particle component}} +/\times \underbrace{C}_{\{\Delta E_k^p;S_k^{\pm pp}\}\text{ varies under } U(\Lambda)}^{\text{Correlations}}$$

- Solving (exactly) the Schr. equation with two unitarily equivalent H leads to
  1. describing the exact same observables, e.g. $\{E_k^\pm, \sigma_k^\pm\}$
  2. extracting two different single-particle shell structures $\{e_p^{\text{cent}}\}$
- Extracting *the* nucleon shell structure from $\{E_k^\pm, \sigma_k^\pm\}$ is an illusory objective
  - One shell structure per (preferably low) resolution scale Λ

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Extract spectroscopic amplitudes [A. M. Mukhamedzhanov, A. S. Kadyrov, PRC82, 051601 (2010)]

- Based on (Λ-dependent) factorization assumption = pure "direct" reaction

$$\sigma_k^{\pm}(\text{exp}) \equiv S_k^{\pm pp}(\text{exp}) \times \sigma_p^{\text{s.p.}}(\text{th})$$

  - Scale Λ only implicit in computation of $\sigma_p^{\text{s.p.}}(\text{th})$
  - Compared to *diagonal* $S_k^{\pm pp}(\text{th})$ from unrelated structure theory
- Should ideally rely on *consistent* structure and reaction *many-body* theories
  1. Define resolution scale Λ, i.e. specify $H(\Lambda)$ used throughout
  2. Validate $\sigma_k^{\pm}(\text{th})$ from many-body reaction theory against $\sigma_k^{\pm}(\text{exp})$
  3. Read off $S_k^{\pm pq}(\Lambda)$ from consistent many-body structure calculation
- How complete $\{S_k^{\pm pq}(\Lambda)\}_{k\in\mathcal{H}_{A\pm1}}$ needs to be to safely reconstruct $e_p^{\text{cent}}(\Lambda)$?

Outline

Error on the reconstruction of ESPEs

Truncated Shell Model calculation in sd shell

1. $V^{2\mathrm{N}}$ = Chiral N^3LO (Λ_χ =500 MeV) + $U(\Lambda)$ down to $\Lambda = 2.2\,\mathrm{fm}^{-1}$
2. Renormalization to $(0d_{5/2}, 0d_{3/2}, 1s_{1/2})$ space through 2^{nd}-order MBPT
3. $e_p^{^{16}0}$ from spherical EDF calculation with Skxtb parameterization

Theoretical "experiment" [A. Signoracci, T. Duguet, unpublished]

1. Truncate Baranger sum rule

$$e_p^{\mathrm{trunc}} \equiv \sum_k^{\mathrm{trunc}} (S_k^{+pp} E_k^{+} + S_k^{-pp} E_k^{-}) / \sum_k^{\mathrm{trunc}} (S_k^{+pp} + S_k^{-pp})$$

   where the truncation relates to

   1. $S_k^{\pm pp} \geq S_{\mathrm{trunc}}^{p}$
   2. $E_k^{\pm} - E_0^{\pm} \leq E_{\mathrm{trunc}}^{\mathrm{Exc}}$

2. Compute error relative to full e_p^{cent}

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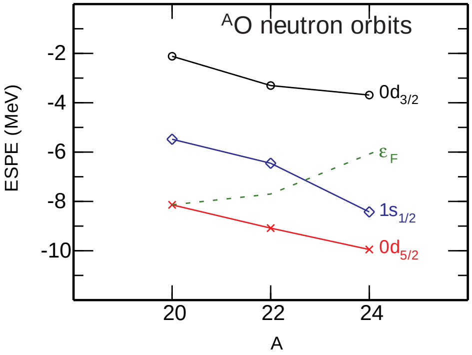
Characterization of Oxygen isotopes



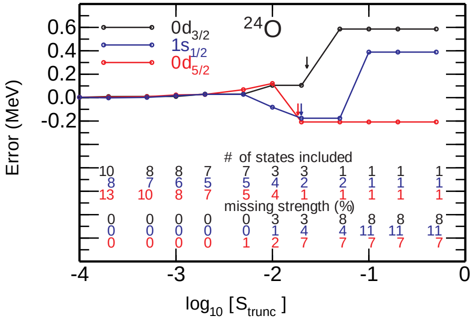
[A. Signoracci, T. Duguet, unpublished]

^{20,22,24}O isotopes

- Evolution of neutron ESPEs

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

ESPE reconstruction in ^{24}O



[A. Signoracci, T. Duguet, unpublished]

Error from S^p_{trunc}

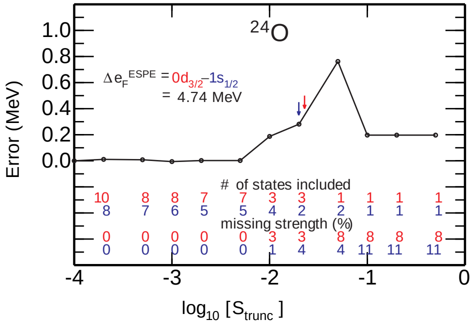
- $0d_{5/2}$, $1s_{1/2}$ and $0d_{3/2}$ ESPEs
- Number of included states
- Missing strength

Using partial spectroscopic strength from one-neutron addition/removal

1. Error on each ESPE can go up to 600 keV
2. 100 keV error requires $S^p_{\text{trunc}} \sim 10^{-2} \Leftrightarrow \sim 95\%$ of the strength $\Leftrightarrow \sim 4$ states
3. Must access the main state from secondary channel ($S^{\pm pp}_k \approx 2.10^{-2}$)
4. Similar in ^{20,22}O but even more necessary to access secondary channel

- Disclaimer: SM = very low scale theory = most favourable scenario

ESPE shell gap in ^{24}O



[A. Signoracci, T. Duguet, unpublished]

Error from S^p_{trunc}

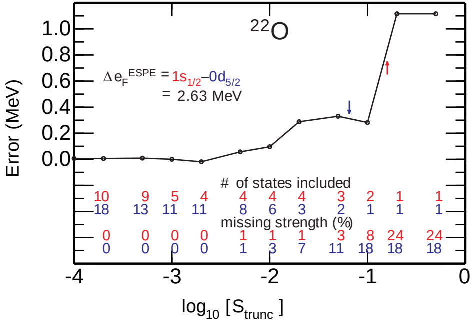
- $0d_{3/2} - 1s_{1/2}$ Fermi gap
- Number of included states
- Missing strength

Using partial spectroscopic strength from one-neutron addition/removal

1. Error on shell gap can be of the order of 800 keV (20%)
2. Sub-leading fragment from primary channel worsen the result at first
3. Main fragments from secondary channel essential

- Disclaimer: SM = very low scale theory = most favourable scenario

ESPE shell gap in ^{22}O



[A. Signoracci, T. Duguet, unpublished]

Error from S^p_{trunc}

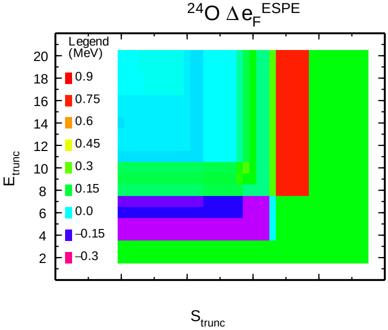
- $1s_{1/2} - 0d_{5/2}$ Fermi gap
- Number of included states
- Missing strength

Using partial spectroscopic strength from one-neutron addition/removal

1. Error on shell gap can be of the order of 1.1 MeV (40%)
2. Trend different from ^{24}O because secondary channel comes in earlier
3. Need to go down to $S^p_{\text{trunc}} \sim 2.10^{-2}$ to reach 10% error

- Disclaimer: SM = very low scale theory = most favourable scenario

ESPE shell gap in ^{24}O



[A. Signoracci, T. Duguet, unpublished]

Error from S^p_{trunc} and $E^{\text{Exc}}_{\text{trunc}}$

- $0d_{3/2} - 1s_{1/2}$ Fermi gap
- Not monotonous in 2D plane
- Targeted accuracy reached for
  1. $S^p_{\text{trunc}} \leq 10^{-2}$
  2. $E^{\text{Exc}}_{\text{trunc}} \approx 8\,\text{MeV}$

Error on ESPE reconstruction must be evaluated

- In practice one (by far) never accesses complete enough reaction data
- One does not simply ignore missing strength but relies on theory
- One must propagate the error associated with the fact that
  1. $\sigma^{\pm}_k(\text{th}) \neq \sigma^{\pm}_k(\text{exp})$ where data available
  2. $\sigma^{\pm}_k(\text{th})$ is not validated where data unavailable

Outline

Correlation between ESPEs and other observables

Partitioning of other observables

$$\overbrace{\underbrace{A}_{E_{2_1^+}}}^{\text{Outcome of Schr. equation}} \equiv \overbrace{\underbrace{B}_{\Delta e_F^{\text{ESPE}}}}^{\text{Ind. particle contribution}} + \overbrace{\underbrace{C}_{\Delta E_{\text{corr.}}}}^{\text{"The rest"}}$$

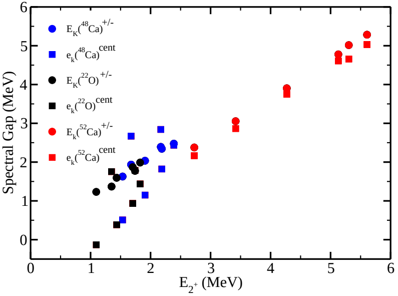
It is sometimes (often?) believed that

1. Correlations contribute minimally to $E_{2_1^+}$ in good closed-shell nuclei
2. The size of A reflects B, i.e.
   - A large $E_{2_1^+}$ reflects a large Δe_F^{ESPE}
   - A low $E_{2_1^+}$ results from a small Δe_F^{ESPE} igniting large correlations

Points of importance

1. This cannot be true in general as B and C can be changed at will
   - See [J. Holt *et al.*, arXiv:1009.5984] for an interesting counter example
2. Revisit in which scheme (i.e. $H(\Lambda)$, many-body method) this is true

Systematic of spectral gap size and $E_{2_1^+}$



Data sample

- $E_0^+ - E_0^-$ and $\Delta e_F^{\mathrm{ESPE}}$ versus $E_{2_1^+}$
- ^{22}O and ^{48,52}Ca
- $\Lambda \in [2.0; 3.0]$ fm^{-1}
- All $SF_0^{\pm}$ involved > 0.9

Pertinence of ESPE spectrum

1. Strong correlation between observable $E_0^+ - E_0^-$ and $E_{2_1^+}$
2. Weaker correlation between $\Delta e_F^{\mathrm{ESPE}}$ and $E_{2_1^+}$
   - No strict causal relationship between both quantities
   - Connection likely to be stronger in restricted valence spaces
   - Dominance of pairing will accentuate this in open shell nuclei

Outline

Take away messages

Single-particle shell structure in (correlated) nuclei

1. Unambiguously defined as eigenvalues of Baranger's centroid matrix
2. Differs significantly from separation energies even in doubly magic nuclei
   - Absolute and relative values differ, ordering may also
   - Approximations add a layer of uncontrollable model dependence
3. Scale-dependent and non-observable
   - Changes with Λ while observables, i.e. $E_k^{\pm}$, $\sigma_k^{\pm}$ or $E_{2_1^+}$, do not
   - Correlation with observables rather weak and Λ dependent
4. Reconstruction from experimental cross sections
   - Requires *consistent* structure and reaction *many-body* theories
   - Secondary channel mandatory *even for good closed-shell nuclei*
   - Must evaluate error associated with missing data and imperfect theory

Manipulating the concept of single-particle shell structure is delicate

Perspectives

Further studies

1. Systematic analysis within truncated shell model

   [A. Signoracci, J. Holt, G. Hagen, T. Duguet, unpublished]

   - Variable valence space size
   - With/without 3N forces

2. Extension of Baranger scheme to particle-number breaking theories

   [V. Somá, T. Duguet, C. Barbieri, PRC84 (2011) 064317]

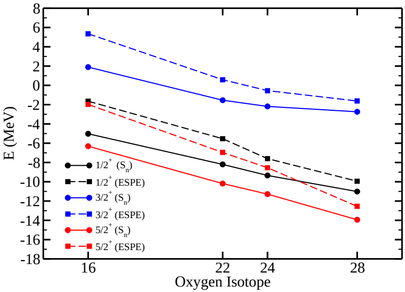
   - Applied to ab-initio self-consistent Gorkov-Green's function theory
   - Systematic access to ESPEs in open-shell nuclei

3. Energy density functional method
   - (SR) Koopman-like theorem with pairing [J. Sadoudi, T. Duguet, unpublished]

     $\Rightarrow$ eigenvalues of $h^{\mathrm{EDF}} \equiv \partial \mathcal{E} / \partial \rho$ are now centroids
   - (MR) ESPEs from sum rule [B. Bally, M. Bender, B. Avez, P.-H. Heenen]

Thank you !

Neutron shell structure evolution



Doubly closed shell O isotopes

- Neutron $E_k^{\pm}$ versus e_p^{cent}
- $\Lambda = 2.4\,\text{fm}^{-1}$

(E_μ^+, E_ν^-) and differ e_p^{cent} from in "good-closed-shell" nuclei

- Difference is not the same in various "good-closed-shell" nuclei
- Difference diminishes strongly going away from N=Z

SM works with perfect closed-shell nucleus, i.e. $e_p^{\text{core}} \equiv E_\mu^+ \, \delta_{pk}$

- Wrong but ok in view of large SF_μ^+ = good effective low-energy d.o.f.