A few things about the nuclear shell structure

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**Question of interest and punch line**

Are there elements of the theory that cannot be fixed by experiment?

- **Realism versus Instrumentalism**
  - An element unambiguously defined within the theory...
  - ... that can be changed at will without changing observables
- True within quantum mechanics and quantum field theory, e.g.
  - **Nuclear shell structure** \( \{e_{nljq}\} \)
  - **Partitioning** \( \vec{J}^g = \vec{S}^g + \vec{L}^g \) of gluon contribution to \( \vec{J}^\text{proton}_{QCD} \)

**Two different levels of model dependency**

- **Within an exact theory** = what we are talking about here
  - \( \{e_{nljq}\} \) from any mean-field approximation is disqualified from the outset!
  - Fundamental model dependency
- **As a result of an approximation** = NOT what we are talking about here
  - Not a fundamental model dependency
  - Very important in practice of course
- Both can cumulate! It is the case for \( \{e_{nljq}\}, \{SF^\pm_k\} \)...
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Nuclear shell structure
## Outline

1. Appropriate definition
2. Non observability
3. Practical reconstruction
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1. Appropriate definition
2. Non observability
3. Practical reconstruction
Key considerations

Motivations to refer to \( \{e_{nljq}\} \)

- Pillar of our understanding
- Drives the quest for exotic nuclei

Problem one actually deals with

Many-body Schroedinger equation

\[
H |\Psi^A_k \rangle = E^A_k |\Psi^A_k \rangle
\]

- One-nucleon addition/removal
  \( E_k^{\pm} \equiv \pm (E_k^{A \pm 1} - E_k^A) \) and \( \sigma_k^{\pm} \)
- Excitations (e.g. \( k \equiv 2^+ \))
  \( \Delta E^A_{0 \rightarrow k} \equiv E^A_k - E^A_0 \) and \( \sigma^A_{0 \rightarrow k} \)

Connection to many-body observable?

Can \( B = \{\epsilon_p\} \) be defined

- only from \( A = \{E_k^{\pm} / |\Psi^A_0 \rangle; |\Psi^A_{k \pm 1} \rangle\} \)?
- not as a zeroth-order approximation!

Partitioning between "uncorrelated contribution" and "correlations"?

Outcome of Schr. equation \( A \)

\[
\begin{aligned}
\{E_k^{\pm} / |\Psi^A_0 \rangle; |\Psi^A_{k \pm 1} \rangle\}
\end{aligned}
\]

\( \iff \)

Ind. particle contribution \( B \)

\[
\{\epsilon_p / |\Phi^A_0 \rangle; |\Phi^A_{p \pm 1} \rangle\}
\]

"The rest" \( C \)

\[
\{\Delta E^p_{k \rightarrow 0} / \delta |\Phi^p_k \rangle\}
\]
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\[ \{\Delta E^p_k / \delta|\Phi^p_k\rangle\} \]
Baranger definition of effective Single-particle energies

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Connection to many-body observable?

[Spectroscopic probability matrices]

\[
S^+_{\mu pq} = \langle \Psi^A_0 | a_p | \Psi^A_{\mu+1} \rangle \langle \Psi^A_{\mu+1} | a_q^\dagger | \Psi^A_0 \rangle \\
S^-_{\nu pq} = \langle \Psi^A_0 | a_q^\dagger | \Psi^A_{-\nu-1} \rangle \langle \Psi^A_{-\nu-1} | a_p | \Psi^A_0 \rangle
\]

[Sum rule and one-body centroid field]

\[
1 = \sum_{\mu} S^+_{\mu} + \sum_{\nu} S^-_{\nu} \\
\hbar^{\text{cent}} = \sum_{\mu} S^+_{\mu} E^+_{\mu} + \sum_{\nu} S^-_{\nu} E^-_{\nu} = T + \Sigma(\infty)
\]

[Spectroscopic factors]

\[
SF^+_\mu \equiv \text{Tr}[S^+_\mu] \\
SF^-_\nu \equiv \text{Tr}[S^-_\nu]
\]

[ESPE]

\[
\hbar^{\text{cent}} \psi^{\text{cent}}_{nljq} = e^{\text{cent}}_{nljq} \psi^{\text{cent}}_{nljq}
\]
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\]

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E_k^\pm \equiv \pm (E_k^{A \pm1} - E_0^A) \quad \text{and} \quad \sigma_k^\pm
\]

- Excitations (e.g. \( k \equiv 2^+ \))
\[
\Delta E_{0 \rightarrow k}^A \equiv E_k^A - E_0^A \quad \text{and} \quad \sigma_{0 \rightarrow k}^A
\]

Spectroscopic factors

\[
S_F^+ = \text{Tr}[S^+], \quad S_F^- = \text{Tr}[S^-]
\]

Sum rule and one-body centroid field

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1 = \sum_\mu S_\mu^+ + \sum_\nu S_\nu^- \\
\hbar^\text{cent} = \sum_\mu S_\mu^+ E_\mu^+ + \sum_\nu S_\nu^- E_\nu^- = T + \Sigma(\infty)
\]

ESPEs in \( ^{74}\text{Ni} \) from Gorkov-SCGF

\[
E_k^\pm [\text{MeV}] \quad \varepsilon_a^\text{cent} [\text{MeV}]
\]

[\( ^{74}\text{Ni} \)]

[\( \text{SF}^\pm \% \)]

[V. Somà, C. Barbieri, T. Duguet, PRC87 (2013) 011303(R)]

ESPE \[\text{[M. Baranger, NPA149 (1970) 225]}\]

\[
\hbar^\text{cent} \psi^\text{cent}_{nljq} = \varepsilon^\text{cent}_{nljq} \psi^\text{cent}_{nljq}
\]

Nuclear shell structure
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Nuclear shell structure
Observable and non observable

Low-energy nuclear many-body problem

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

  Hamiltonian \( H \equiv \sum_\nu H^{(\nu)} \)

  \( \begin{align*}
  H |\Psi_k^A\rangle &= E_k^A |\Psi_k^A\rangle \\
  \end{align*} \)

Self-adjoint operator \( O \equiv \sum_\nu O^{(\nu)} \)

\( \begin{align*}
  O_k^A &= \langle \Psi_k^A | O |\Psi_k^A\rangle \\
  \end{align*} \)

General unitary transformation \( U(s) \) over Fock space

- \( H(s) \equiv U(s) H U^\dagger(s) \) leads to
  \( \begin{align*}
  H(s) |\Psi_k^A(s)\rangle &= E_k^A |\Psi_k^A(s)\rangle \\
  |\Psi_k^A(s)\rangle &= U(s) |\Psi_k^A\rangle \\
  \end{align*} \)

- Observable \( O(s) \equiv U(s) O U^\dagger(s) \) leads to
  \( \langle \Psi_k^A(s) | O(s) |\Psi_k^A(s)\rangle = O_k^A \)

- Not transforming operator \( O \) defines a non-observable quantity as
  \( \partial_s \langle \Psi_k^A(s) | O |\Psi_k^A(s)\rangle \neq 0 \)

Nuclear shell structure
Low-energy nuclear many-body problem

- A-body problem defined within a consistent EFT at a given order in $(Q/\Lambda)$

  Hamiltonian
  \[ H \equiv \sum_\nu H^{(\nu)} \]
  \[ \Rightarrow \left\{ \begin{array}{l}
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- General unitary transformation $U(s)$ over Fock space

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  \[ \begin{array}{l}
  H(s) |\Psi_k^A(s)\rangle = E_k^A |\Psi_k^A(s)\rangle \\
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- Not transforming operator $O$ defines a non-observable quantity as
  \[ \partial_s \langle \Psi_k^A(s) | O | \Psi_k^A(s) \rangle \neq 0 \]
Scale dependence of ESPEs

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

- **RG flow for operators and states**
  
  $$\frac{d}{ds} O(s) \equiv [\eta(s), O(s)]$$
  
  where
  
  $$\eta(s) \equiv \frac{dU(s)}{ds} U^+(s) = -\eta^+(s)$$

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

- **RG flow for the quantities of interest**

  $$\frac{d}{ds} S^{-pq}_\nu(s) = -\langle \Psi^A_0(s) | [\eta(s), a_p^\dagger] | \Psi^{A-1}_\nu(s) \rangle \langle \Psi^{A-1}_\nu(s) | a_q | \Psi^A_0(s) \rangle$$

  $$-\langle \Psi^A_0(s) | a_p^\dagger | \Psi^{A-1}_\nu(s) \rangle \langle \Psi^{A-1}_\nu(s) | [\eta(s), a_q] | \Psi^A_0(s) \rangle \neq 0$$

  $$\frac{d}{ds} E^{-}_\nu(s) = 0$$

  $$\frac{d}{ds} h^\text{cent}_{pq}(s) = -\langle \Psi^A_0(s) | \{[\eta(s), a_p], H(s) \}, a_q^\dagger \} + \{[a_p, H(s)], [\eta(s), a_q^\dagger] \} | \Psi^A_0(s) \rangle \neq 0$$

- Keeping amplitudes invariant would require to use

  $$U(s)a_p^\dagger U^+(s) = \sum_q u^p_q(s) a_q^\dagger + \sum_{qrs} u^p_{qrs}(s) a_q^\dagger a_r a_s + \ldots$$

  in their definition and would thus kill the original purpose.
Non-observable nature and its consequences

**Unitary transformation** $H(2) = U^\dagger H(1) U$


**Observable**
- $E_k^\pm (1) = E_k^\pm (2)$
- $\sigma_k^\pm (1) = \sigma_k^\pm (2)$

**Not observable**
- $e_a^{\text{cent}}(1) \neq e_a^{\text{cent}}(2)$
- $SF_k^\pm (1) \neq SF_k^\pm (2)$


**Partitioning of observable**

<table>
<thead>
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<th>Many-body observable</th>
<th>Single-particle component</th>
<th>Correlations</th>
</tr>
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<tbody>
<tr>
<td>$\tilde{E}_\mu^+$</td>
<td>$\sum_a s_\mu^{+a} e_a^{\text{cent}}$</td>
<td>$\sum_{pq} s_\mu^{+pq} \Sigma_{qp}^\text{dyn} (E_\mu^+)$</td>
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Invariant under $U$
- Varies under $U$

**Extracting the shell structure from** $\{E_k^\pm, \sigma_k^\pm\}$ **is an illusory objective**

- Two practitioners using the same (exact) many-body theory with $H(1)$ and $H(2)$
  - will reproduce the observables $\{E_k^\pm, \sigma_k^\pm\}$ identically (and exactly)
  - will extract two different single-particle shell structures $e_a^{\text{cent}}(1) \neq e_a^{\text{cent}}(2)$
- Still useful to give one interpretation of reality (must agree on "gauge", e.g. $H(1)$)

**Invariant under** $U$
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$s_\mu^+ \equiv S_\mu^+ / SF_\mu^+$

$\Sigma_{\mu}^{\text{dyn}}(\omega) \equiv \Sigma(\omega) - \Sigma(\infty)$
Non-observable nature and its consequences

Unitary transformation $H(2) = U^\dagger H(1) U$  

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Partitioning of observable

Many-body observable $\left\{ E_{\mu}^+, \sigma_{\mu}^{\pm} \right\}$

\[ E_{\mu}^+ = \sum_a s_{\mu}^{+aa} e_{a}^{\text{cent}} + \sum_{pq} s_{\mu}^{+pq} \Sigma_{pq}^{\text{dyn}} (E_{\mu}^+) \]

\( \Sigma_{\text{dyn}}(\omega) \equiv \Sigma(\omega) - \Sigma(\infty) \)

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1. Appropriate definition

2. Non observability

3. Practical reconstruction
Protocol to reconstruct $e_{a}^{\text{cent}}$?

**Definition**

$S_{k}^{\pm}$ are *intrinsically* theoretical objects

- Only defined when $H$ is specified *together with a fixed "gauge"
- Data only "fix" $H$ up to $U^\dagger U = 1$, i.e. data cannot fix $S_{k}^{\pm}$

**Usual approach**

- Hypothesis of pure direct reaction
  
  $\sigma_{k}^{\pm}\,(\text{exp}) \equiv S_{k}^{\pm pp} \times \sigma_{p}^{\text{s.p.}}\,(\text{th})$

- Only defines *diagonal* part of $S_{k}^{\pm}$

- $\sigma_{p}^{\text{s.p.}}\,(\text{th})$ not consistent with structure calc.

- Validity of factorization "gauge" dependent

**Towards a more appropriate protocol**

- Postulate consistent theoretical scheme
  
  - $H$ with fixed "gauged" used throughout

- Consistent structure/reaction theory
  
  - Validate theory against $E_{k}^{\pm}\,(\text{exp})/\sigma_{k}^{\pm}\,(\text{exp})$

- Read $S_{k}^{\pm}$ off structure calculation

**Two questions of interest once the theoretical scheme is fixed**

- What is the error on $e_{p}^{\text{cent}}$ due to truncated strength

- What is the (statistical) theoretical uncertainty on $e_{p}^{\text{cent}}$ due to incomplete $E_{k}^{\pm}\,(\text{exp})/\sigma_{k}^{\pm}\,(\text{exp})$
Protocol to reconstruct $\epsilon_a^{\text{cent}}$?

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Protocol to reconstruct $e_{d}^{\text{cent}}$?

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Theoretical experiment based on SM in sd shell

Protocol

1. Perform full sd shell calculation to simulate reference (pseudo-) data
2. Choose subset as "experimentally known" (pseudo-) data
3. Compute $\chi^2$ to "known" (pseudo-) data and propagate statistical uncertainty

[A. Signoracci, T. Duguet, in preparation]

I. Error due to plain truncation of strength

- **Truncate Baranger sum rule in $^{20,22,24}$O**

$$ e_{a}^{\text{trunc}} \equiv \frac{\sum_{S_{F_{k}}} S_{k}^{+} \geq S_{\text{trunc}} (S_{k}^{+} + S_{k}^{-})}{\sum_{S_{F_{k}}} S_{k}^{+} \geq S_{\text{trunc}} (S_{k}^{+} + S_{k}^{-})} $$

- Error on Fermi gap up to 20 % (800 keV)
- Error on SO splitting up to 13 % (800 keV)
- Mandatory to include in doubly-magic $^{24}$O

Main fragment in secondary channel

Strength down to $\sim 10^{-2}$

Error on $0d_{5/2} - 0d_{3/2}$ SO splitting in $^{24}$O

Error (MeV) vs. $\log_{10} [S_{\text{trunc}}]$ graph: 

$\delta_{0d_{5/2} - 0d_{3/2}} = 6.26$ MeV

Missing strength in $^{24}$O:

- # of states included
- Missing strength (%)
Theoretical experiment based on SM in sd shell

**Protocol**

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**II. Theoretical (statistical) uncertainty**

- Full strength provided by (uncertain) theory
- Incomplete data available to validate theory

\[ \chi^2 = \sum_{i,j \in \text{known}} (E_i^{\text{th}} - E_i^{\text{exp}}) V_{ij}^{-1} (E_j^{\text{th}} - E_j^{\text{exp}}) \]

- Propagate $1\sigma$ uncertainty from $\chi^2_{\text{min}} + 1$
- Assess impact of newly measured data
- Systematic uncertainty comes on top
- Protocol to be applied to real exp.

**Uncertainty on Fermi gap in $^{24}\text{O}$**

![Graph showing uncertainty on Fermi gap in $^{24}\text{O}$]
Conclusions

Take-away messages

1. The shell structure depends on the theoretical scheme, i.e. "gauge", used
   - Link to observables and interpretation change with "gauge"

2. This does not prevent one from linking behaviour of observables to ESPEs
   - As long as the theoretical scheme used is stated and consistent

3. Uncertainties must be evaluated and stated
   - One can anticipate impact of newly measured data
Scale dependence of ESPEs in CC calculations

**Non-absoluteness of ESPEs**

- Scale dependence of $E_\nu^-$ from omitted induced forces and clusters
- Intrinsic scale dependence of $\epsilon_p^{\text{cent}} \approx 6$ MeV for $s \in [2.0, 3.0]$ fm$^{-1}$
  - Not identical for all shells
- 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]

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**One-neutron removal in $^{24}$O**

- $E^-_\nu$ and $\epsilon_p^{\text{cent}}$ versus $s$
- $s \in [2.0; 3.0]$ fm$^{-1}$