

A few things about the nuclear shell structure

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Nuclear Structure and Astrophysical Applications, July 8-12 2013, ECT*

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 $\{e_{nljq}\}$
 [T. Duguet, G. Hagen, PRC85 (2012) 034330 ; T. Duguet, *Thèse d'Habilitation* (2012)]
 - Partitioning $\vec{J}^g = \vec{S}^g + \vec{L}^g$ of gluon contribution to $\vec{J}_{QCD}^{\text{proton}}$
 [C. Lorcé, hep-ph/arXiv:1306.0456]

Two different levels of model dependency

- ① 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
- ② As a result of an approximation = NOT what we are talking about here
 - Not a fundamental model dependency
 - Very important in practice of course
- ③ Both can cumulate! It is the case for $\{e_{nljq}\}, \{SF_k^\pm\} \dots$

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Outline

- 1 Appropriate definition
- 2 Non observability
- 3 Practical reconstruction

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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

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

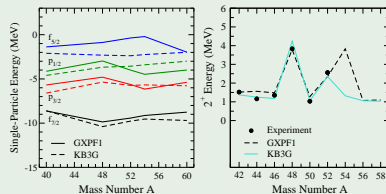
- One-nucleon addition/removal

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

- Excitations (e.g. $k \equiv 2_1^+$)

$$\Delta E_{0 \rightarrow k}^A \equiv E_k^A - E_0^A \quad \text{and} \quad \sigma_{0 \rightarrow k}^A$$

Connection to many-body observable?



[J. D. Holt, *et al.*, JPG39 (2012) 085111]

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

- ⦿ only from $A = \{E_k^\pm / |\Psi_0^A\rangle; |\Psi_k^{A\pm 1}\rangle\}$?
- ⦿ not as a zeroth-order approximation!

Partitioning between "uncorrelated contribution" and "correlations"?

$$\underbrace{\text{Outcome of Schr. equation}}_A \quad \overset{?}{\iff} \quad \underbrace{\text{Ind. particle contribution}}_B \quad + \quad \underbrace{\text{"The rest"}}_C$$

$$\underbrace{\{E_k^\pm / |\Psi_0^A\rangle; |\Psi_k^{A\pm 1}\rangle\}}_A \quad \iff \quad \underbrace{\{\epsilon_p / |\Phi_0^A\rangle; |\Phi_p^{A\pm 1}\rangle\}}_B \quad + \quad \underbrace{\{\Delta E_k^p / \delta |\Phi_k^p\rangle\}}_C$$

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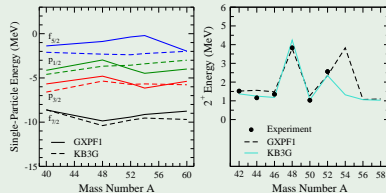
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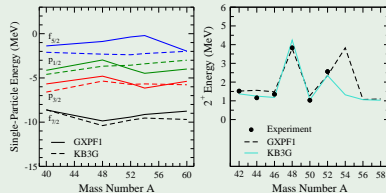
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Baranger definition of effective Single-particle energies

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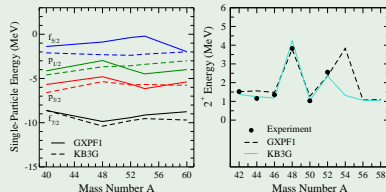
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Spectroscopic probability matrices

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

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

Spectroscopic factors

$$SF_\mu^+ \equiv \text{Tr}[S_\mu^+]$$

$$SF_\nu^- \equiv \text{Tr}[S_\nu^-]$$

Sum rule and one-body centroid field

$$\mathbf{1} \equiv \sum_\mu S_\mu^+ + \sum_\nu S_\nu^-$$

$$\mathbf{h}^{\text{cent}} \equiv \sum_\mu S_\mu^+ E_\mu^+ + \sum_\nu S_\nu^- E_\nu^- = \mathbf{T} + \mathbf{\Sigma}(\infty)$$

ESPE [M. Baranger, NPA149 (1970) 225]

$$\mathbf{h}^{\text{cent}} \psi_{nljq}^{\text{cent}} \equiv e_{nljq}^{\text{cent}} \psi_{nljq}^{\text{cent}}$$

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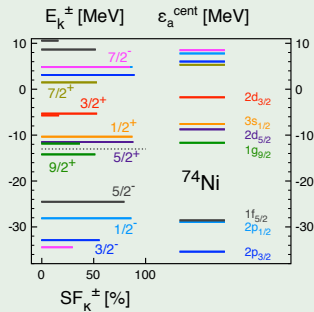
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ESPEs in ^{74}Ni from Gorkov-SCGF



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

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Observable and non observable

Low-energy nuclear many-body problem

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

$$\left. \begin{array}{l} \text{Hamiltonian } H \equiv \sum_{\nu} H^{(\nu)} \\ \text{Self-adjoint operator } O \equiv \sum_{\nu} O^{(\nu)} \end{array} \right\} \implies \left\{ \begin{array}{l} H |\Psi_k^A\rangle = E_k^A |\Psi_k^A\rangle \\ O_k^A = \langle \Psi_k^A | O | \Psi_k^A \rangle \end{array} \right.$$

- 2 General unitary transformation $U(s)$ over Fock space

- 1 $H(s) \equiv U(s) H U^\dagger(s)$ leads to $\left\{ \begin{array}{l} H(s) |\Psi_k^A(s)\rangle = E_k^A |\Psi_k^A(s)\rangle \\ |\Psi_k^A(s)\rangle \equiv U(s) |\Psi_k^A\rangle \end{array} \right.$

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

- 3 Not transforming operator O defines a non-observable quantity as

$$\partial_s \langle \Psi_k^A(s) | O | \Psi_k^A(s) \rangle \neq 0$$

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Scale dependence of ESPEs

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

- 1 RG flow for operators and states

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

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

- 2 RG flow for the quantities of interest

$$\frac{d}{ds}S_v^{-pq}(s) = -\langle\Psi_0^A(s)|[\eta(s), a_p^\dagger]|\Psi_v^{A-1}(s)\rangle\langle\Psi_v^{A-1}(s)|a_q|\Psi_0^A(s)\rangle$$

$$-\langle\Psi_0^A(s)|a_p^\dagger|\Psi_v^{A-1}(s)\rangle\langle\Psi_v^{A-1}(s)|[\eta(s), a_q]|\Psi_0^A(s)\rangle \neq 0$$

$$\frac{d}{ds}E_v^-(s) = 0$$

$$\frac{d}{ds}h_{pq}^{\text{cent}}(s) = -\langle\Psi_0^A(s)|\{[\eta(s), a_p], H(s)\}, a_q^\dagger\} + \{[a_p, H(s)], [\eta(s), a_q^\dagger]\}|\Psi_0^A(s)\rangle \neq 0$$

- 3 Keeping amplitudes invariant would require to use

$$U(s)a_p^\dagger U^\dagger(s) = \sum_q u_q^p(s)a_q^\dagger + \sum_{qrs} u_{qrs}^p(s)a_q^\dagger a_r^\dagger a_s + \dots$$

in their definition **and would thus kill the original purpose**

Non-observable nature and its consequences

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

[T. Duguet and G. Hagen, PRC 85 (2012) 034330]

Observable

✓ $E_k^\pm(1) = E_k^\pm(2)$

✓ $\sigma_k^\pm(1) = \sigma_k^\pm(2)$

Not observable

✗ $e_a^{\text{cent}}(1) \neq e_a^{\text{cent}}(2)$

✗ $SF_k^\pm(1) \neq SF_k^\pm(2)$

For SF_k^\pm see [R. J. Furnstahl, H. W. Hammer, PLB 531 (2002) 203 ; B. K. Jennings (2011), arXiv:1102.3721]

Partitioning of observable

[T. Duguet, unpublished]

$$\underbrace{E_\mu^+}_{\text{Invariant under } U} = \underbrace{\sum_a s_\mu^{+aa} e_a^{\text{cent}}}_{\text{Varies under } U} + \underbrace{\sum_{pq} s_\mu^{+pq} \Sigma_{qp}^{\text{dyn}}(E_\mu^+)}_{\text{Varies under } U}$$

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

$$s_\mu^+ \equiv S_\mu^+ / SF_\mu^+$$

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 $H(2)$
 - ① will reproduce the observables $\{E_k^\pm, \sigma_k^\pm\}$ identically (and exactly)
 - ② 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. $H(1)$)

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Many-body observable = Single-particle component + Correlations

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Protocol to reconstruct e_a^{cent} ?

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

- 1 Postulate consistent theoretical scheme
 - 1 H with fixed "gauge" used throughout
 - 2 Consistent structure/reaction theory
- 2 Validate theory against $E_k^\pm(\text{exp})/\sigma_k^\pm(\text{exp})$
- 3 Read S_k^\pm off structure calculation

Two questions of interest once the theoretical scheme is fixed

- 1 What is the error on e_p^{cent} due to truncated strength
- 2 What is the (statistical) theoretical uncertainty on e_p^{cent} due to incomplete $E_k^\pm(\text{exp})/\sigma_k^\pm(\text{exp})$

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Theoretical experiment based on SM in sd shell

Protocol

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

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

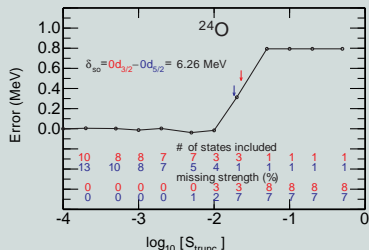
I. Error due to plain truncation of strength

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

$$e_a^{\text{trunc}} \equiv \frac{\sum_{SF_k^\pm \geq S_{\text{trunc}}} (S_k^{+aa} E_k^+ + S_k^{-aa} E_k^-)}{\sum_{SF_k^\pm \geq S_{\text{trunc}}} (S_k^{+aa} + S_k^{-aa})}$$

- 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
 - 1 Main fragment in secondary channel
 - 2 Strength down to $\sim 10^{-2}$

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



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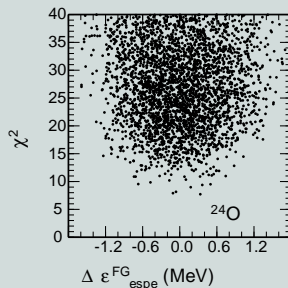
II. Theoretical (statistical) uncertainty

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

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

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

Uncertainty on Fermi gap in ^{24}O

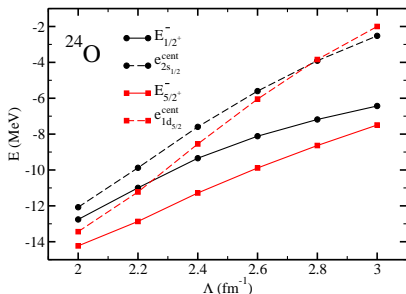


Conclusions

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



One-neutron removal in ^{24}O

■ E_y^- and e_p^{cent} versus s

■ $s \in [2.0; 3.0] \text{ fm}^{-1}$

Non-absoluteness of ESPEs

- ① Scale dependence of E_y^- from omitted induced forces and clusters
- ② Intrinsic scale dependence of $e_p^{cent} \approx 6 \text{ MeV}$ for $s \in [2.0, 3.0] \text{ fm}^{-1}$
 - 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]