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

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Outline

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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

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

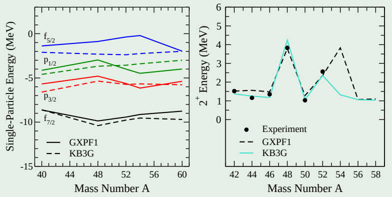
- One-nucleon addition/removal

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

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

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

Connection to many-body observable?



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

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

1. only from $A = \{E_k^{\pm} / |\Psi_0^A\rangle; |\Psi_k^{A\pm1}\rangle\}$?
2. not as a zeroth-order approximation?

Partitioning between "uncorrelated contribution" and "correlations"?

$$\underbrace{A}_{\{E_k^{\pm}/|\Psi_0^A\rangle;|\Psi_k^{A\pm1}\rangle\}} \overset{?}{\Longleftrightarrow} \underbrace{B}_{\{\epsilon_p/|\Phi_0^A\rangle;|\Phi_p^{A\pm1}\rangle\}} + \underbrace{C}_{\{\Delta E_k^p/\delta|\Phi_k^p\rangle\}}$$

Outcome of Schr. equation — Ind. particle contribution — "The rest"

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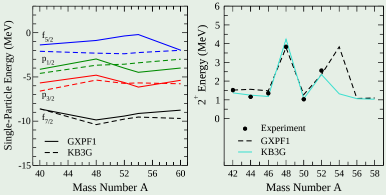

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Outcome of Schr. equation		Ind. particle contribution		"The rest"
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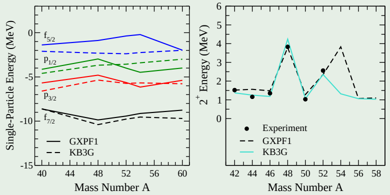

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Outcome of Schr. equation (A) — Ind. particle contribution (B) — "The rest" (C)

Baranger definition of effective Single-particle energies

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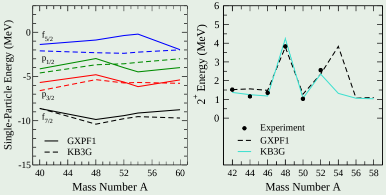

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Spectroscopic probability matrices

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

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

Spectroscopic factors

$$SF_\mu^+ \equiv \text{Tr}[\mathbf{S}_\mu^+]$$

$$SF_\nu^- \equiv \text{Tr}[\mathbf{S}_\nu^-]$$

Sum rule and one-body centroid field

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

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

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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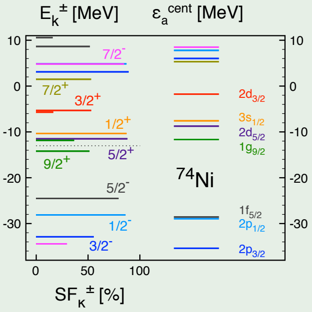
ESPEs in ^{74}Ni from Gorkov-SCGF



[V. Somà, C. Barbieri, T. Duguet, arXiv:1208.2472]

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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 $(Q/\Lambda_\chi)^\nu$

$$\left.\begin{array}{ll}\text{Hamiltonian} & H \equiv \sum_\nu H^{(\nu)} \\ \text{Other operator} & O \equiv \sum_\nu O^{(\nu)}\end{array}\right\} \Longrightarrow \left\{\begin{array}{l} H|\Psi^A_k\rangle = E^A_k|\Psi^A_k\rangle \\ O^A_k = \langle\Psi^A_k|O|\Psi^A_k\rangle\end{array}\right.$$

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

   1. $H(s) \equiv U(s)\,H\,U^\dagger(s)$ leads to $\left\{\begin{array}{l} H(s)|\Psi^A_k(s)\rangle = E^A_k|\Psi^A_k(s)\rangle \\ |\Psi^A_k(s)\rangle \equiv U(s)|\Psi^A_k\rangle\end{array}\right.$
   2. Observable $O(s) \equiv U(s)\,O\,U^\dagger(s)$ leads to $\langle\Psi^A_k(s)|O(s)|\Psi^A_k(s)\rangle = O^A_k$
   3. Not transforming operator O defines a non-observable quantity as

$$\partial_s\langle\Psi^A_k(s)|O|\Psi^A_k(s)\rangle \neq 0$$

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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

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

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

2. RG flow for the quantities of interest

$$\frac{d}{ds} S^{-pq}_\nu(s) = -\langle\Psi^{\text{A}}_0(s)| [\eta(s), a^\dagger_p] |\Psi^{\text{A-1}}_\nu(s)\rangle \langle\Psi^{\text{A-1}}_\nu(s)| a_q |\Psi^{\text{A}}_0(s)\rangle - \langle\Psi^{\text{A}}_0(s)| a^\dagger_p |\Psi^{\text{A-1}}_\nu(s)\rangle \langle\Psi^{\text{A-1}}_\nu(s)| [\eta(s), a_q] |\Psi^{\text{A}}_0(s)\rangle \neq 0$$

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

$$\frac{d}{ds} h^{\text{cent}}_{pq}(s) = -\langle\Psi^{\text{A}}_0(s)| \{[[\eta(s), a_p], H(s)], a^\dagger_q\} + \{[a_p, H(s)], [\eta(s), a^\dagger_q]\} |\Psi^{\text{A}}_0(s)\rangle \neq 0$$

3. Keeping amplitudes invariant would require to use

$$U(s) a^\dagger_p U^\dagger(s) = \sum_q u^p_q(s) a^\dagger_q + \sum_{qrs} u^p_{qrs}(s) a^\dagger_q a^\dagger_r a_s + \ldots$$

in their definition and would thus kill the original purpose

Non-observable nature and its consequences

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

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

(Many-body observable = Single-particle component + Correlations)

$$\mathbf{\Sigma}^{\text{dyn}}(\omega) \equiv \mathbf{\Sigma}(\omega) - \mathbf{\Sigma}(\infty)$$
$$\mathbf{s}_\mu^+ \equiv \mathbf{S}_\mu^+ / SF_\mu^+$$

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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Protocol to reconstruct e_a^{cent}?

$\mathbf{S}_k^{\pm}$ 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 $\mathbf{S}_k^{\pm}$

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 $\mathbf{S}_k^{\pm}$
- $\sigma_p^{\text{s.p.}}(\text{th})$ not consistent with structure calc.
- Validity of factorization "gauge" dependent

Towards a more appropriate protocol

1. Postulate consistent theoretical scheme
   1. H with fixed "gauged" used throughout
   2. Consistent structure/reaction theory
2. Validate theory against $E_k^{\pm}(\text{exp})/\sigma_k^{\pm}(\text{exp})$
3. Read $\mathbf{S}_k^{\pm}$ 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. Randomize $\sim 10^4$ interactions and compute χ^2 to "known" (pseudo-) data

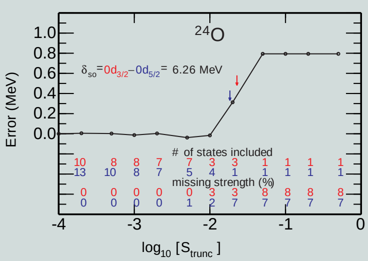
I. Error due to plain truncation of strength

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

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

- 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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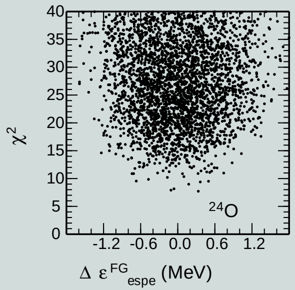
II. Theoretical (statistical) uncertainty

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

Uncertainty on Fermi gap in ^{24}O

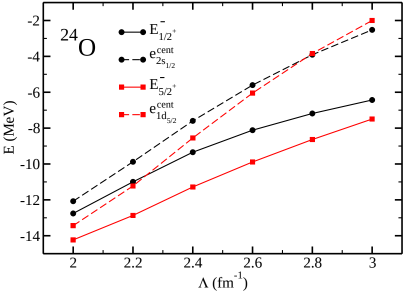


Conclusions

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^-_ν and e^{cent}_p versus s
- $s \in [2.0; 3.0]$ fm^{-1}

Non-absoluteness of ESPEs

1. Scale dependence of E^-_ν from omitted induced forces and clusters
2. Intrinsic scale dependence of $e^{cent}_p \approx 6$ MeV for $s \in [2.0, 3.0]$ 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]