Non-observable nature of the nuclear shell structure
Meaning, illustrations and consequences

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T. D., G. Hagen, PRC 85 (2012) 034330
T. D., H. Hergert, J. D. Holt, V. Somà, PRC 92 (2015) 034313

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Outline

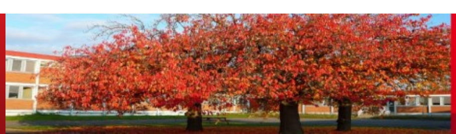
I. Punchline

II. Why do we refer to the one-nucleon shell structure?

III. Model-independent definition

IV. Non-observable nature

V. Illustrations from ab-initio many-body calculations



Question of interest and punchline

Are there (mandatory) 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**

No counterpart in the empirical world

This is the case within quantum mechanics and quantum field theory, e.g.

- **Gauge dependence of gluon contributions to proton spin ½?**

  [C. Lorcé, NPA 925C , 1 (2014) ; M. Wakamatsu, arXiv:1409.4474; F. Wang *et al*., arXiv:1411.0077]

- **Scale/scheme dependence of parton distributions factorization**

  [G. Sterman *et al*., RMP 67, 157 (1995)]

- **Scale/scheme dependence of single-nucleon shell energies, spectroscopic factors…**

One thing that must be made clear

Mathematical representation embedded in a "Surplus structure"

[M. Redhead, in *Symmetries in Physics: Philosophical Reflections*, K. Brading & E. Castellani (eds.), 2003]

Considerations within EXACT quantum mechanics = *what we are talking about here*

- **Fundamental feature of the many-body problem**
- **Single-nucleon energies from mean-field are disqualified from the outset**

Effects of approximations = *NOT what we are talking about here*

- **Crucial in practice but come on top of the above considerations**

The single-nucleon shell structure

Epistemic role

Interacting quantum many-body problem

Motivation to refer to the shell structure

- **Pillar of our understanding**
- **Provides convenient simplified picture**

Problem one actually deals with

Many-body Schrödinger equation

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

- **One-nucleon addition/removal**

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

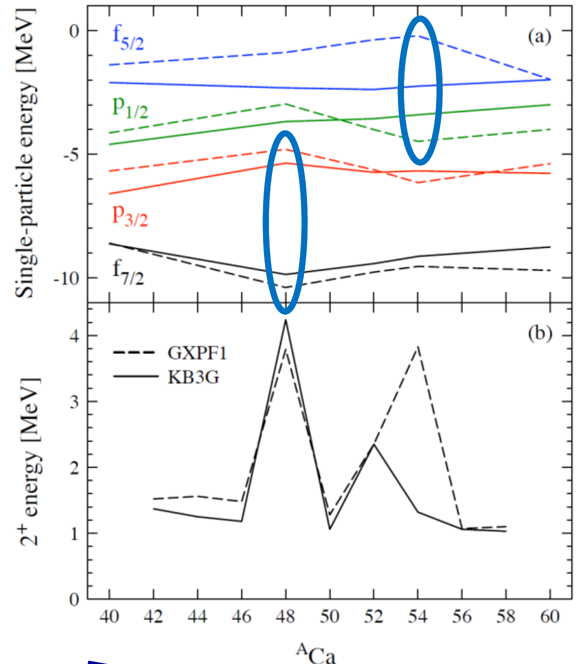
- **Excitations , e.g. k=2_1^+**

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

Partitioning of observable, e.g., separation energy

$$\underbrace{E_k^{\pm}}_{\text{Schr. equation}} = \underbrace{e_p}_{\text{Ind. particles}} + \underbrace{\Delta E_{p\to k}}_{\text{Correlations}}$$

Connection to many-body observables?



Empirical *fp* shell model calculation

2_1^+ versus ESPE Fermi gap?

- **"Common wisdom" says yes**
- **Seems indeed to be true**
- **Is that it?**

Look for observables/systems where this dominates
i.e. where the shell structure leaves its "fingerprints"

Interacting quantum many-body problem

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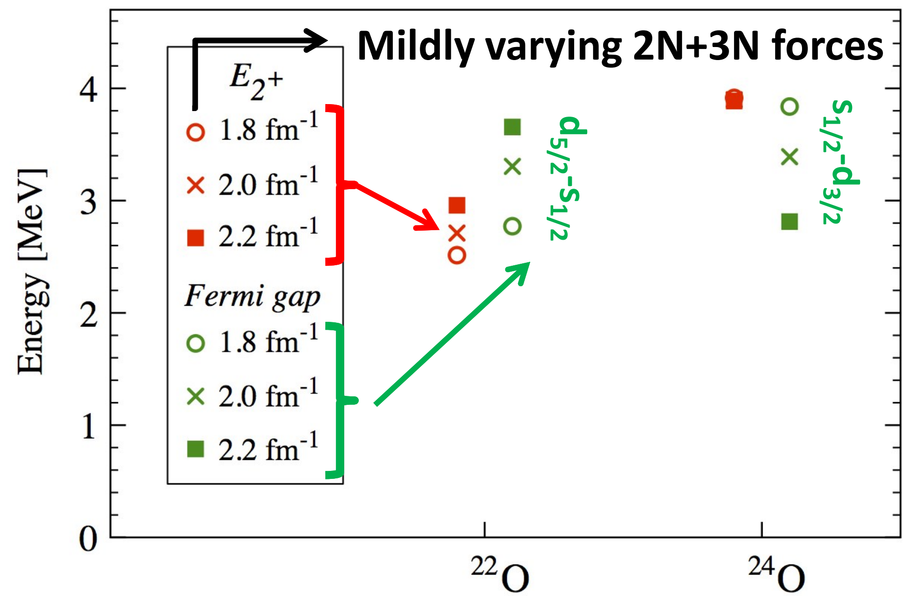
Connection to many-body observables?

Microscopic *sd* shell model calculation of ^{22,24}O



① Observable E_{2+} essentially unchanged

② Larger change of ESPE Fermi gap

Correlations depend on Hamiltonian!?

→ Inequivalent Hamiltonians?

→ Fundamental feature?

Part II

The single-nucleon shell structure

Model-independent definition

Definition of nucleon shell energies

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

$$SF_\mu^+ \equiv \sum_p S_\mu^{+pp}$$
$$SF_\nu^- \equiv \sum_p S_\nu^{-pp}$$

s.p. occupations

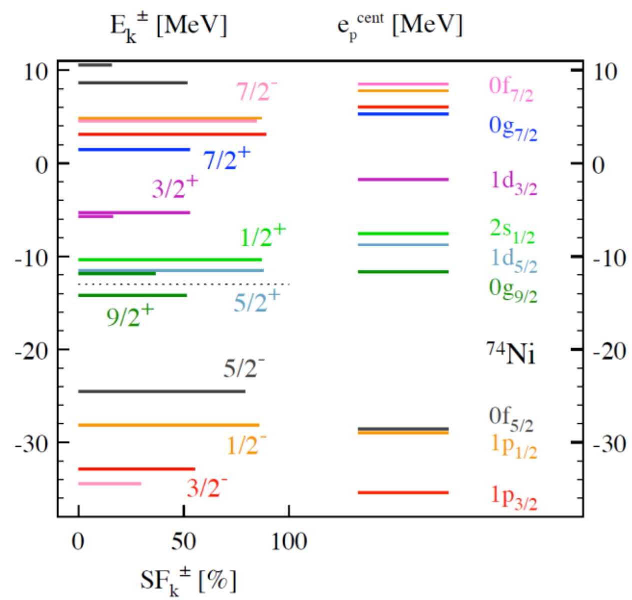
$$1 - n_p \equiv \sum_\mu S_\mu^{+pp}$$
$$n_p \equiv \sum_\nu S_\nu^{-pp}$$

Sum rule and 1-body centroid field

$$\mathbf{1} \equiv \sum_\mu \mathbf{S}_\mu^+ + \sum_\nu \mathbf{S}_\nu^-$$
$$\mathbf{h}^{\text{cent}} \equiv \sum_\mu \mathbf{S}_\mu^+ E_\mu^+ + \sum_\nu \mathbf{S}_\nu^- E_\nu^- = \mathbf{T} + \mathbf{\Sigma}(\infty)$$

Energy-*independent* part of the one-nucleon self energy

ESPEs in ^{74}Ni from Gorkov-SCGF



Effective single-particle energies (ESPE)

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

1. **Defined solely from outputs of the many-body Schrödinger Eq.**
2. **Computable in *any* many-body scheme, i.e. SM, ab initio etc**
3. **Independent of the single-particle basis used**
4. **Weighted average of one-nucleon separation energies**
5. **Physically relates to the averaged dynamics of nucleons**
6. **Reduce to HF s.p. energies in HF approximation**

[M. Baranger, NPA149 (1970) 225]

Part III

The single-nucleon shell structure

Non-observable nature

Non-observable nature of ESPEs - 1

The nuclear many-body problem as a low-energy chiral effective field theory

$$O \equiv \sum_{\nu} O_{(\nu)} \equiv O^{1N} + O^{2N} + \ldots + O^{AN}$$ **Self-adjoint operator at a given order in $(Q/\Lambda_\chi)^\nu$**

$$H\,|\Psi_k^A\rangle = E_k^A\,|\Psi_k^A\rangle$$ **Schrodinger equation for the Hamiltonian**

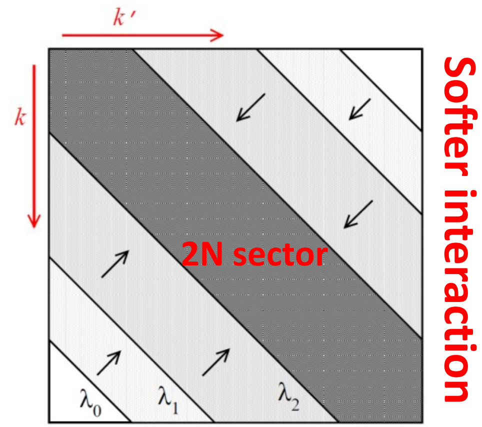
$$O_{kk'}^{AA'} = \langle \Psi_k^A | O | \Psi_{k'}^{A'} \rangle$$ **Amplitudes for other operators**

Unitary (similarity renormalization group) transformation over Fock space

$$\begin{aligned} O(\lambda) &\equiv U(\lambda)\, O\, U^\dagger(\lambda) \\ &\equiv O^{1N}(\lambda) + O^{2N}(\lambda) + O^{3N}(\lambda) + \ldots \end{aligned}$$

Induces higher-body interactions

$$\begin{cases} H(\lambda)|\Psi_\mu^A(\lambda)\rangle = E_k^A |\Psi_\mu^A(\lambda)\rangle \\ |\Psi_\mu^A(\lambda)\rangle \equiv U(\lambda)\,|\Psi_\mu^A\rangle \end{cases}$$



[S.K. Bogner et al., PPNP 65, 94 (2010)]

Observables are invariant under the transformation

$$\frac{d}{d\lambda} E_k^A(\lambda) = 0 \qquad \frac{d}{d\lambda} \sigma^{A_k + B_l \rightarrow C_m + D_n}(\lambda) = 0$$

cea

cea
ESNT

Non-observable nature of ESPEs - 2

Behavior of nucleon shell energies under the transformation

$$U_\mu^p(\lambda) \equiv \left\langle \Psi_0^A(\lambda) \middle| a_p \middle| \Psi_\mu^{A+1}(\lambda) \right\rangle$$

$$V_\nu^p(\lambda) \equiv \left\langle \Psi_0^A(\lambda) \middle| a_p^\dagger \middle| \Psi_\nu^{A\text{-}1}(\lambda) \right\rangle$$

Operator not transformed BY DEFINITION

$$\frac{d}{d\lambda} \mathbf{S}_\mu^+(\lambda) \neq 0 \quad \text{and} \quad \frac{d}{d\lambda} \mathbf{S}_\nu^-(\lambda) \neq 0$$

In spite of $\frac{d}{d\lambda} E_\nu^-(\lambda) = \frac{d}{d\lambda} E_\mu^+(\lambda) = 0$

Sum rule invariant

$$\frac{d}{d\lambda}\left[\sum_\mu \mathbf{S}_\mu^+(\lambda) E_\mu^+(\lambda) + \sum_\nu \mathbf{S}_\nu^-(\lambda) E_\nu^-(\lambda)\right] \neq 0$$

$$\frac{d}{d\lambda}\left[\sum_\mu \mathbf{S}_\mu^+(\lambda) + \sum_\nu \mathbf{S}_\nu^-(\lambda)\right] = 0$$

ESPEs run with λ

Nucleon shell energies can be changed while leaving observables untouched

$$\frac{d}{d\lambda} e_{nljq}^{\text{cent}}(\lambda) \neq 0$$

Transformation law derived (not given here)

Same for

$$SF_\mu^+ \equiv \sum_p S_\mu^{+pp} \qquad 1 - n_p \equiv \sum_\mu S_\mu^{+pp}$$

$$SF_\nu^- \equiv \sum_p S_\nu^{-pp} \qquad n_p \equiv \sum_\nu S_\nu^{-pp}$$

Key consequences - 1

There exist intrinsically theoretical objects $\mathbf{S}^{\pm}_{\mu}(\lambda),\, SF^{\pm}_{\mu}(\lambda),\, e^{\text{cent}}_{nljq}(\lambda)\ldots$

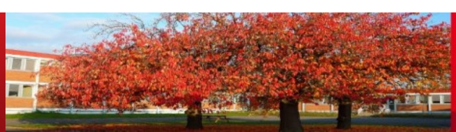
- **Empirical data only "fix" *H* up to** $U^{\dagger}\,U = 1$
- **Nothing fixes the shell structure in the empirical world**
- **Must agree on arbitrary λ to fix** $e^{\text{cent}}_{nljq}(\lambda)$ **and establish correlations with observables**

Exact partitioning of observable one-nucleon separation energies

$$\underbrace{\overset{\text{Many-body observable}}{E^{+}_{\mu}}}_{\text{Invariant under } U} = \underbrace{\overset{\text{Single-particle component}}{\sum_{a} s^{+aa}_{\mu}\; e^{\text{cent}}_{a}}}_{\text{Varies under } U} + \underbrace{\overset{\text{Correlations}}{\sum_{pq} s^{+pq}_{\mu}\; \Sigma^{\text{dyn}}_{qp}(E^{+}_{\mu})}}_{\text{Varies under } U}$$

The partitioning is scale dependent
Convenient scale may maximize ESPE component
Will not be valid in absolute terms though

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



Key consequences – 2

Test case: Analysis of complete (ideal) one-nucleon transfer experiments $\{\sigma_k^{\pm}, E_k^{\pm}\}$

Hyp. A: Practitioners 1 and 2 have EXACT many-body structure & reactions theories at hand

Hyp. B: Practitioners 1/2 uses Hamiltonian $H(\lambda_1)/H(\lambda_2)$ such that $H(\lambda_1) = U^{+} H(\lambda_2)\, U$

Practitioner 1 $\{\sigma_k^{\pm}(\lambda_1), E_k^{\pm}(\lambda_1), SF_k^{\pm}(\lambda_1), e_p^{\text{cent}}(\lambda_1)\}$

Practitioner 2 $\{\sigma_k^{\pm}(\lambda_2), E_k^{\pm}(\lambda_2), SF_k^{\pm}(\lambda_2), e_p^{\text{cent}}(\lambda_2)\}$

Same PHYSICS

$$\sigma_k^{\pm}(\lambda_1) = \sigma_k^{\pm}(\lambda_2)$$

$$E_k^{\pm}(\lambda_1) = E_k^{\pm}(\lambda_2)$$

But different INTERPRETATION

$$e_p^{\text{cent}}(\lambda_1) \neq e_p^{\text{cent}}(\lambda_2)$$

$$SF_k^{\pm}(\lambda_1) \neq SF_k^{\pm}(\lambda_2)$$

- **Practitioners *must* find different ESPEs/SFs**
- **Interpretation is not absolute**
- **Must agree on a scheme to compare**
- **Approximations come on top**

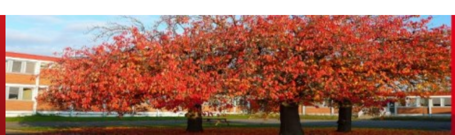
No sense a priori to compare, e.g.

$$SF_k^{\pm} \equiv \frac{\sigma_k^{\pm}(exp)}{\sigma_p^{s.p.}(\lambda)}$$ **and** $SF_k^{\pm}(\lambda')$ **From e.g. SM**

Need to work at a consistent λ (can change λ)
For which factorization is valid
Use for other processes (if factorization valid)

Further conclusion for the years to come

Focus on *consistency* rather than *accuracy* to combine/develop structure & reactions



Results from ab-initio calculations

Many-body methods

- Gorkov-SCGF ADC(2)

  [V. Somà, T. D., C. Barbieri, PRC 84, 064317 (2011)]
- MR-IMSRG(2)

  [H. Hergert et al., PRL 110, 242501 (2013)]

Unitary SRG transformation U(λ)

- Variation λ = 1.88, 2.00, 2.24 fm^{-1}

Set up

- N^3LO 2NF (Λ_{2N} = 500 MeV/c)
  [A. Ekstrom *et al.*, PRL 110, 192502 (2013)]
- Local N^2LO 3NF (Λ_{3N} = 400 MeV/c)
  [P. Navrátil, FBS 41, 117 (2007)]
- HO basis
  - N_{1max} = 14 and 15
  - N_{2max} = 28 and 30
  - N_{3max} = 16 and 14

Breaking unitarity of SRG transformation U(λ)

Origin

1. Omit $V^{AN}(\lambda)$ for A>3
2. Not exact solving of Schr. Eq.

Consequence

Artificial λ dependence of observables

Need to characterize it before looking at non observables

Tests in oxygen isotopes

1. Omit or keep $V^{3N}(\lambda)$
2. HFB vs Gorkov-SCGF(2) and MR-IMSRG(2)

Artificial λ dependence of total binding energies

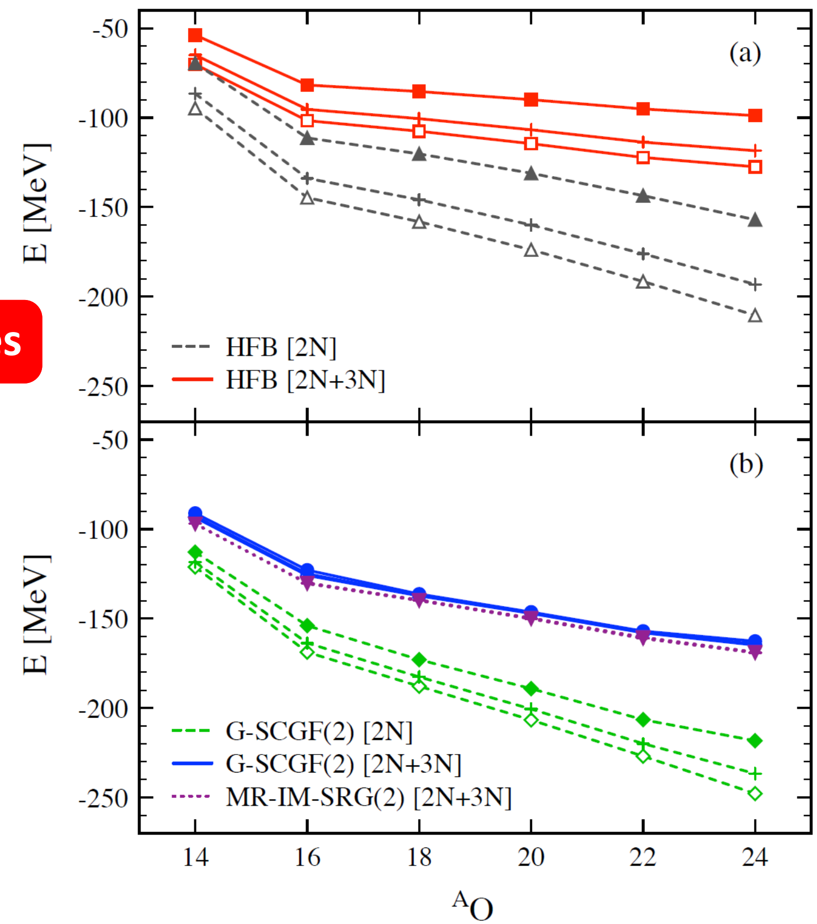
Strongly reduced by

- keeping $V^{3N}(\lambda)$
- Going to Gorkov-SCGF(2) and MR-IMSRG(2)

By a factor ~25 down to 2MeV (G-SCGF)

By a factor ~100 down to 0.5MeV (IM-SRG)

Oxygen isotopes



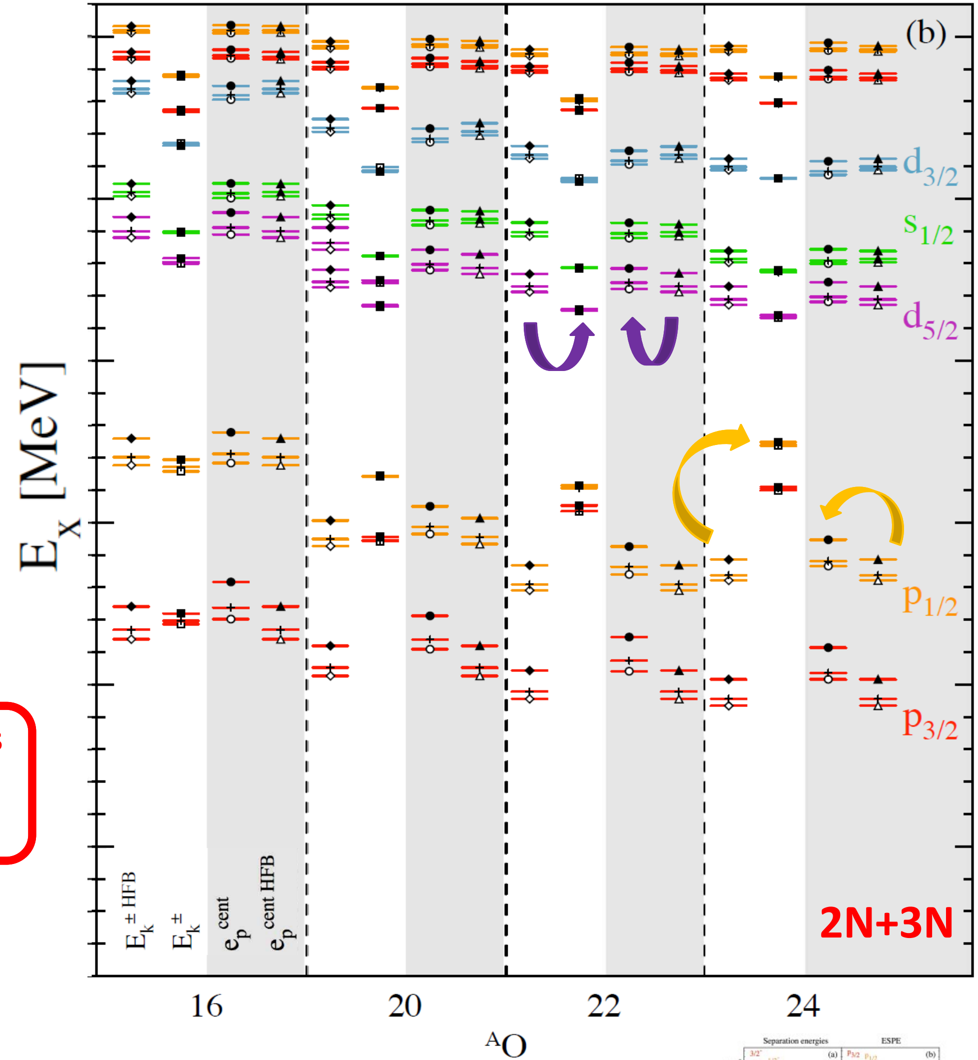
Non-observable shell structure

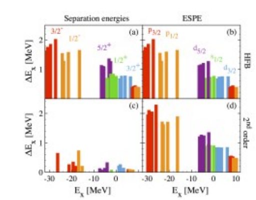
λ dependence

From HFB to Gorkov-SCGF(2)

1. ***E_k^{+-}* spread reduced very significantly**
2. **ESPE spread UNCHANGED**
3. **Correlations impact former much more**
   1. **Compression of E_k^{+-} spectrum**
   2. **No compression in ESPE spectrum**

One-nucleon separation energies
vs
Effective single-particle energies





Non-observable shell structure

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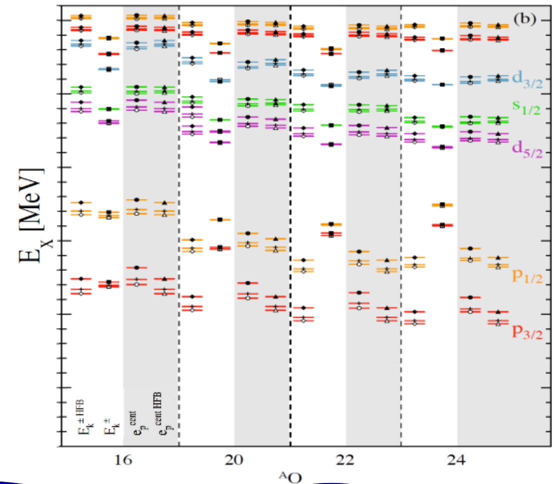
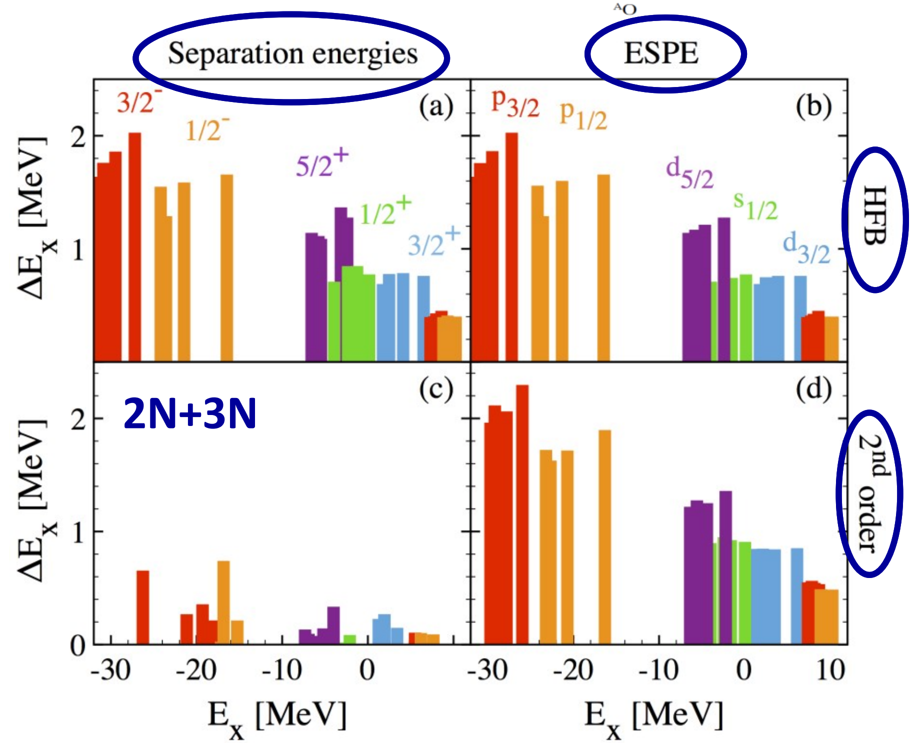


Systematically and quantitatively true

1. **$<\Delta E_k^{+-}>$ = 0.2 MeV**
2. **<ΔESPE> = 1.1 MeV**

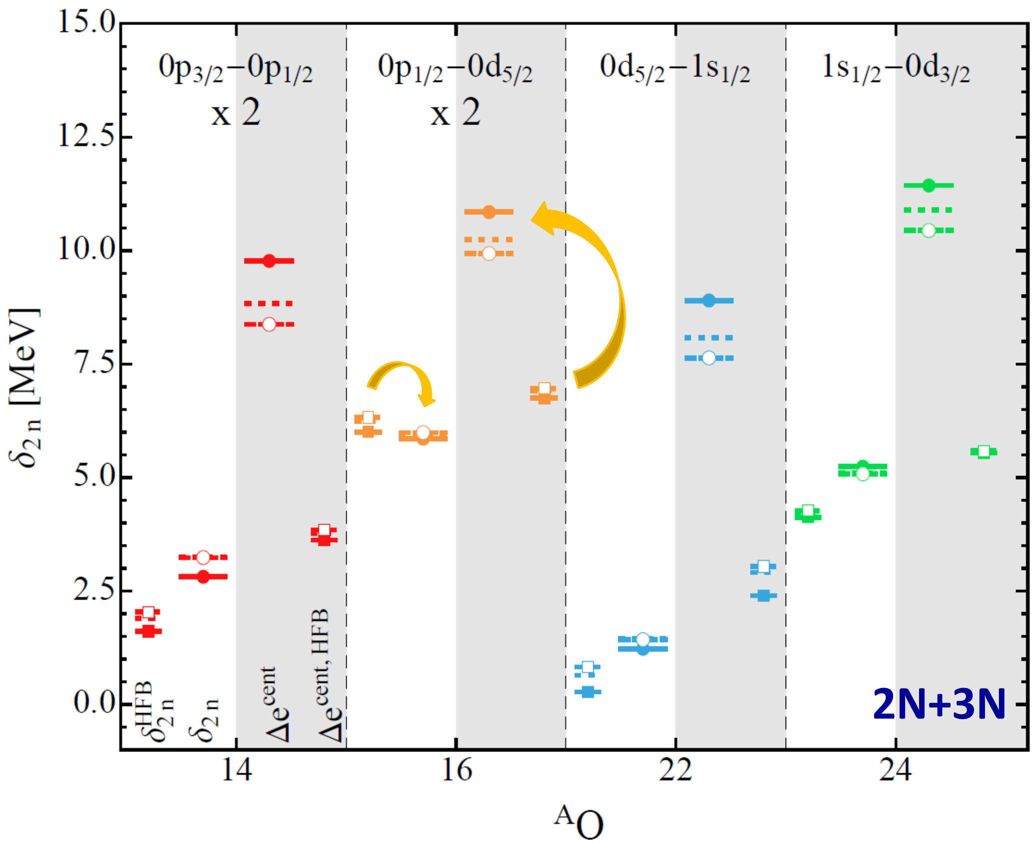
Will be further reduced by

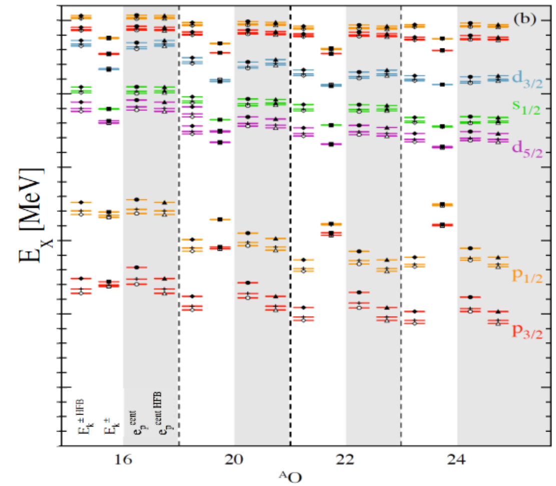
1. **Keeping $V^{AN}(\lambda)$ for A>3**
2. **Improving many-body convergence**

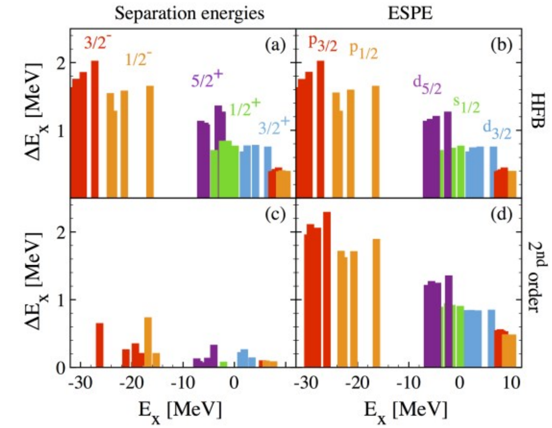


Non-observable shell structure

Two-neutron shell gap vs ESPE Fermi gap







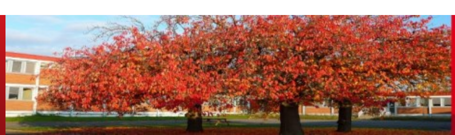
$$\delta_{2n}(N,Z) \equiv \frac{1}{2}\left[E(N+2,Z) - 2E(N,Z) + E(N-2,Z)\right]$$

vs

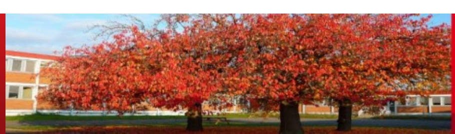
$$\Delta e_F^{cent}(N,Z) \equiv e_p^{cent}(N,Z) - e_h^{cent}(N,Z)$$

Results

1. **All previous conclusions remain valid**
2. Δe_F^{cent} **not a good measure for used λ values**



Conclusions and perspectives



Conclusions and perspectives

Conclusions

The single-nucleon shell structure is a non-observable quantity

- **Similar for SFs, correlations, wave-functions…**

These quantities provide a *scale/scheme dependent* interpretation of observables

- **Often based on explicit or implicit factorization/partitioning theorems**
- **Ex: simple factorization of many-body cross section for direct processes**
- **Ex: simple partitioning of one-nucleon separation energies , two-nucleon shell gaps**

Some perspectives

Make scale/scheme explicit and use consistently

Factorization/partitioning of observables in terms of non observables

- **Validity often depends on scale**
- **Within valid domain the running with scale can be used**
- **Use for other observables for which factorization is valid**

Must develop *consistent* structure and reaction many-body theories

- **To revisit/develop factorization/partitioning theorems**
- **Identify quantitatively kinematical regime of validity**