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, arXiv:1411.1237 (to be published in PRC)

Workshop on *Theory for open-shell nuclei near the limits of stability*

May 11th –29th 2015, NSCL/FRIB, MSU

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*

- **Applies to any implementation scheme of quantum many-body problem**
- **Analysis invokes Baranger's model-independent definition of ESPE**

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

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

Part I

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**

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

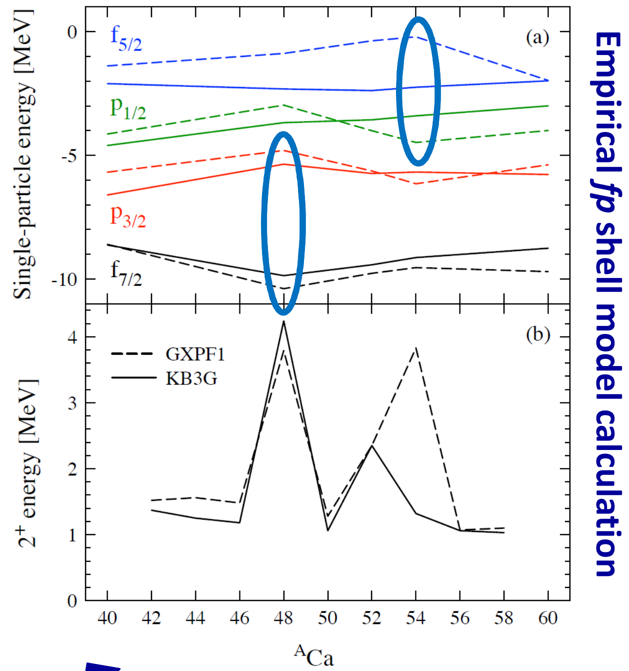
- **Excitations , e.g. k=2_1^+**

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

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?



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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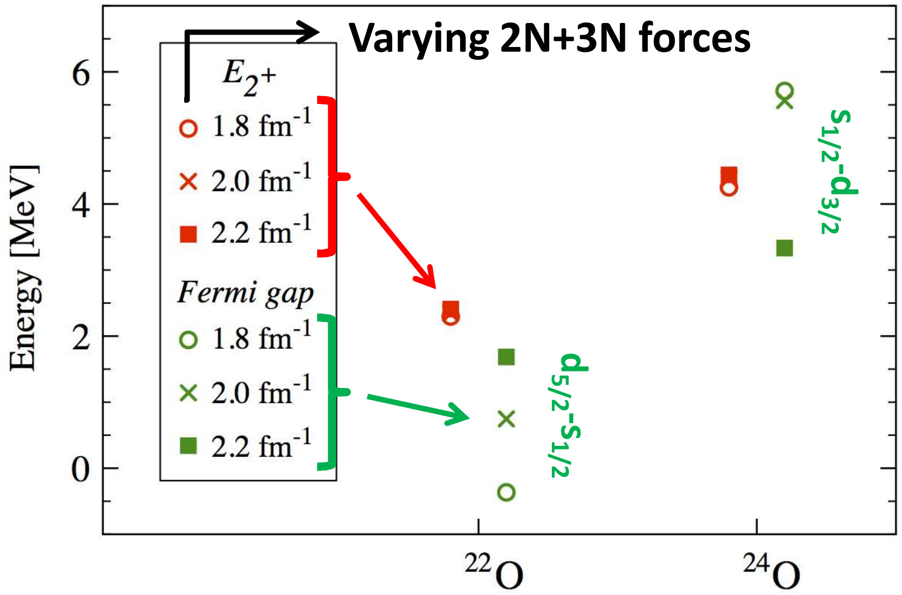
Connection to many-body observables?

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



① Observable E_{2+} essentially unchanged

② Significant change of ESPE Fermi gap

Connection depends on Hamiltonian!?

→ Inequivalent Hamiltonians?

→ Fundamental feature?

The single-nucleon shell structure

Model-independent definition

Definition of nucleon shell energies

Spectroscopic probability matrices

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

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

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

Effective single-particle energies (ESPE)

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

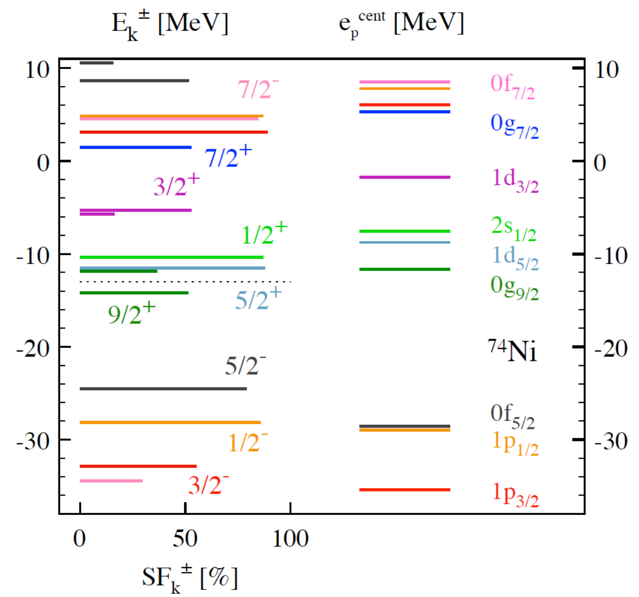
[M. Baranger, NPA149 (1970) 225]

Spectroscopic factors

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

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

ESPEs in ^{74}Ni from Gorkov-SCGF



1. Defined solely from outputs of the 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

The single-nucleon shell structure

Non-observable nature

Non-observable nature of ESPEs - 1

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

$$O \equiv \sum_{\nu} O_{(\nu)} \equiv O^{1\mathrm{N}} + O^{2\mathrm{N}} + \ldots + O^{\mathrm{AN}}$$

Self-adjoint operator at a given order in $(Q/\Lambda_\chi)^\nu$

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

Schrodinger equation for the Hamiltonian

$$O^{\mathrm{AA'}}_{kk'} = \langle\Psi^{\mathrm{A}}_k|\,O\,|\Psi^{\mathrm{A'}}_{k'}\rangle$$

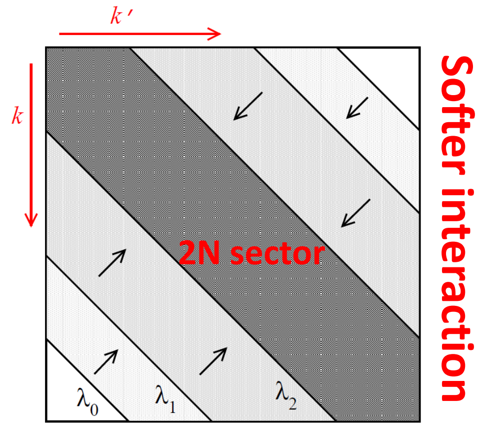
Amplitudes for other operators

Unitary (e.g. similarity renormalization group) transformation over Fock space

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

Induces higher-body interactions

$$\begin{cases} H(\lambda)|\Psi^{\mathrm{A}}_{\mu}(\lambda)\rangle = E^{\mathrm{A}}_{k}|\Psi^{\mathrm{A}}_{\mu}(\lambda)\rangle \\ |\Psi^{\mathrm{A}}_{\mu}(\lambda)\rangle \equiv U(\lambda)\,|\Psi^{\mathrm{A}}_{\mu}\rangle \end{cases}$$



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

Observables are invariant under the transformation

$$\frac{d}{d\lambda}E^{\mathrm{A}}_k(\lambda) = 0 \qquad \frac{d}{d\lambda}\sigma^{A_k+B_l\to C_m+D_n}(\lambda) = 0$$

Non-observable nature of ESPEs - 2

Behavior of nucleon shell energies under the transformation

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

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

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

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

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

Transformation law derived (not given here)

Nucleon shell energies can be changed while leaving observables untouched

Same for $\begin{cases} SF_\mu^+ \equiv \mathrm{Tr}[\mathbf{S}_\mu^+] \\ SF_\nu^- \equiv \mathrm{Tr}[\mathbf{S}_\nu^-] \end{cases}$

Key consequences - 1

There exist intrinsically theoretical quantities $\mathbf{S}_{\mu}^{\pm}(\lambda),\ SF_{\mu}^{\pm}(\lambda),\ e_{nljq}^{\mathrm{cent}}(\lambda)\ldots$

- **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** $e_{nljq}^{\mathrm{cent}}(\lambda)$ **and establish correlations with observables**

Exact partitioning of observable one-nucleon separation energies

$$\overset{\text{Many-body observable}}{\underbrace{E_{\mu}^{+}}_{\text{Invariant under } U}} = \overset{\text{Single-particle component}}{\underbrace{\sum_{a} s_{\mu}^{+aa}\; e_{a}^{\mathrm{cent}}}_{\text{Varies under } U}} + \overset{\text{Correlations}}{\underbrace{\sum_{pq} s_{\mu}^{+pq}\; \Sigma_{qp}^{\mathrm{dyn}}(E_{\mu}^{+})}_{\text{Varies under } U}}$$

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

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

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 scheme/scale to compare**
- **Approximations come on top**

No sense a priori to compare, e.g.

$SF_k^{\pm} \equiv \dfrac{\sigma_k^{\pm}(exp)}{\sigma_p^{s.p.}(\lambda)}$ **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^{3}LO 2NF (Λ_{2N} = 500 MeV/c)
  [D. R. Entem, R. Machleidt PRC 68, 041001 (2003)]
- Local N^{2}LO 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

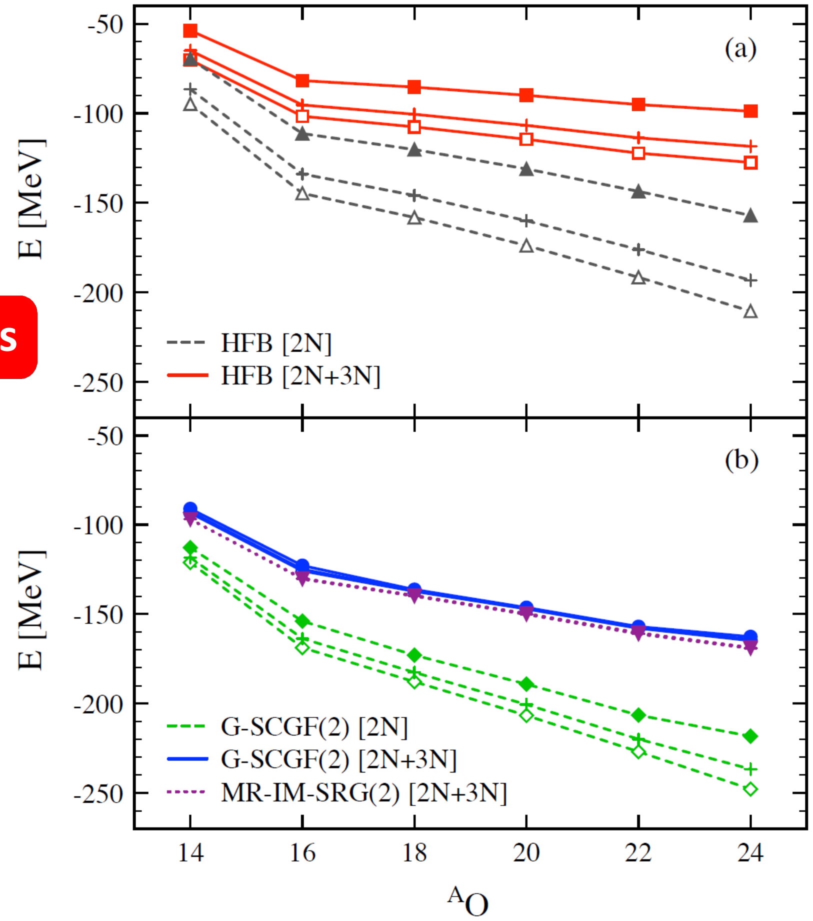
1. Omit or keep $V^{3N}(\lambda)$
2. HFB vs Gorkov-SCGF(2) and MR-IMSRG(2)

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 ~15 down to 2MeV (G-SCGF)
By a factor ~60 down to 0.5MeV (IM-SRG)

Oxygen isotopes



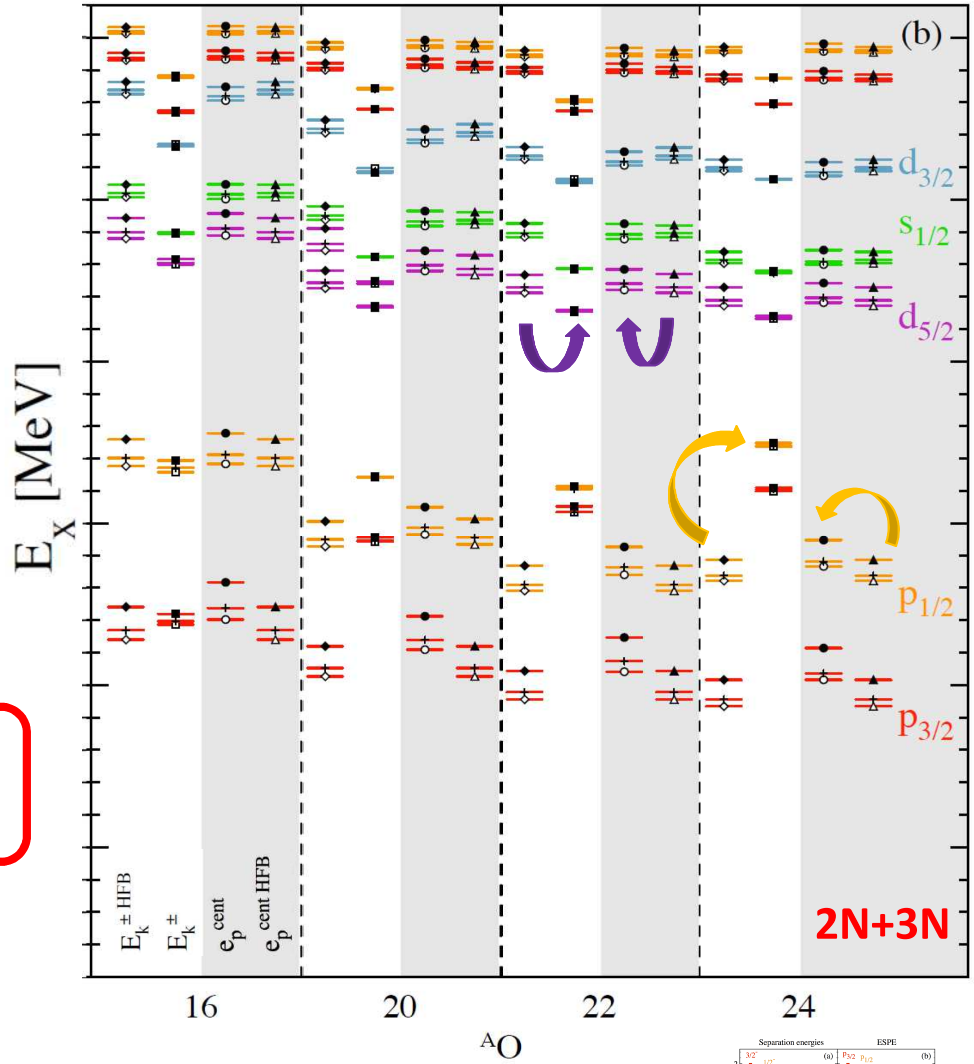
Non-observable shell structure

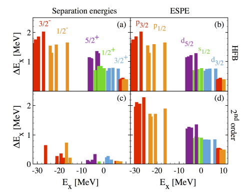
λ dependence

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





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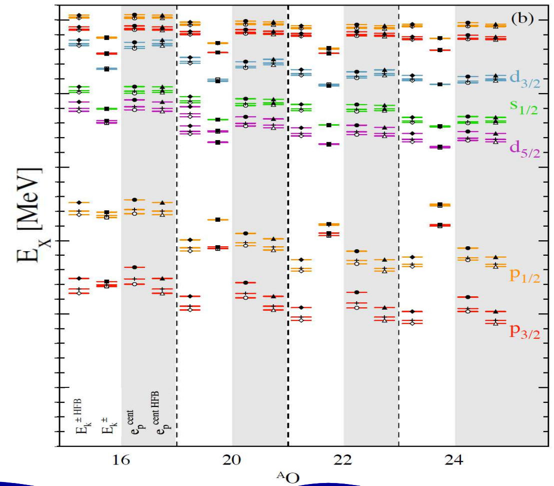
    1. **Compression of *E_k^{+-}* spectrum**
    2. **No compression in ESPE spectrum**

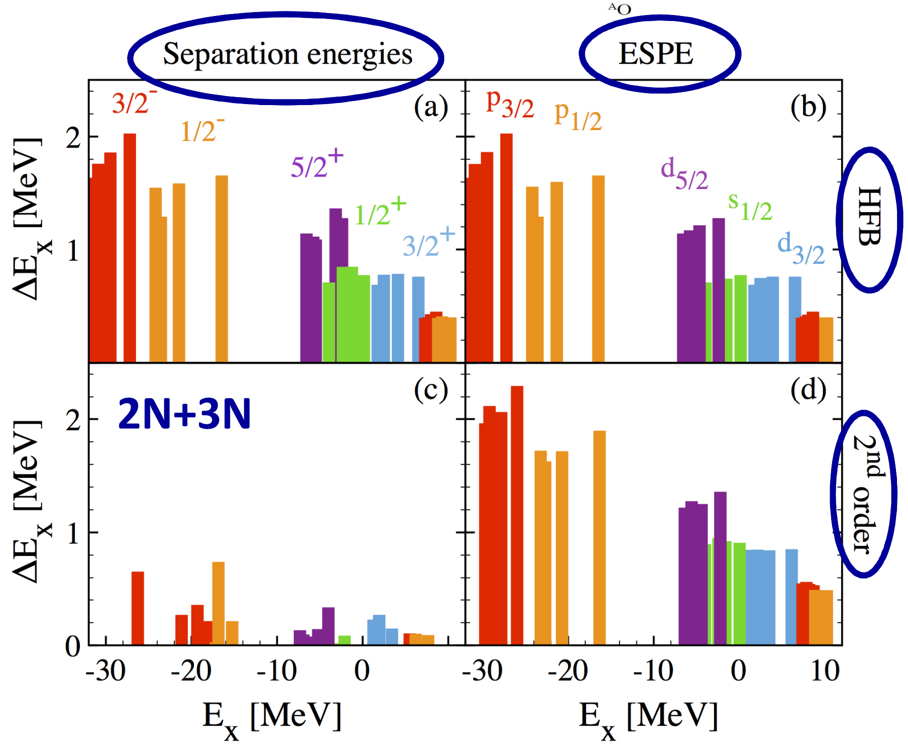
Systematically and quantitatively true

1. **$\langle \Delta E_k^{+-} \rangle$ = 0.2 MeV**
2. **$\langle \Delta \mathrm{ESPE} \rangle$ = 1.1 MeV**

Will be further reduced by

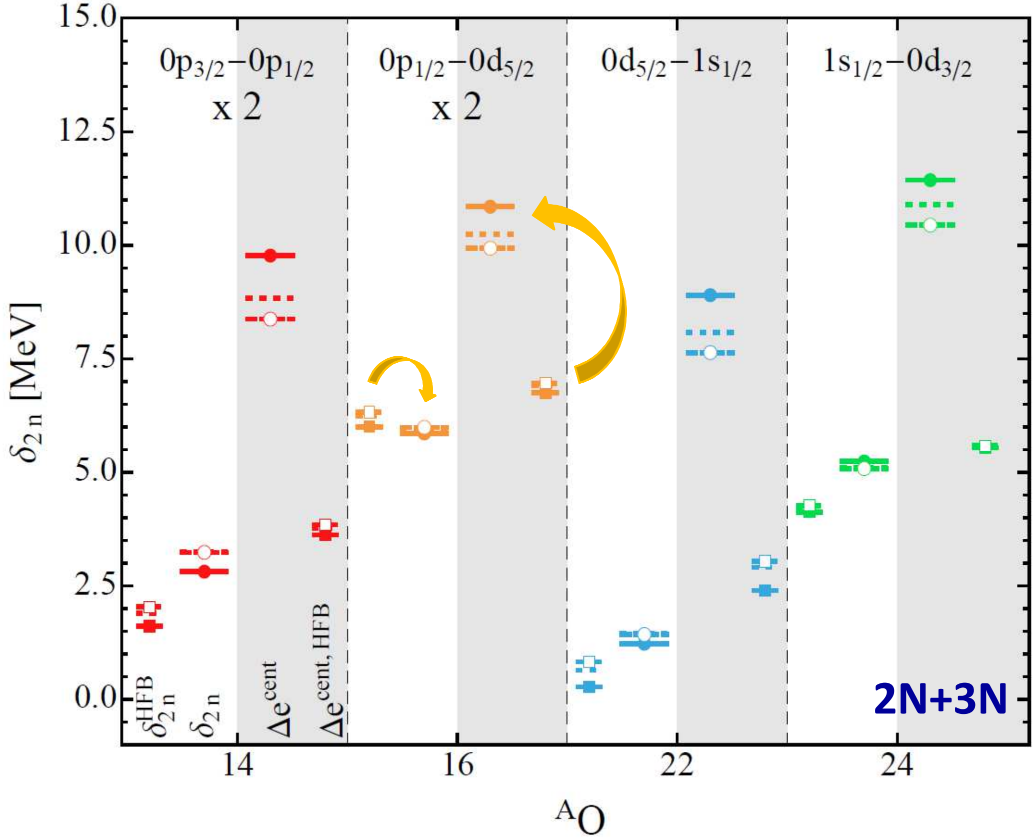
1. **Keeping $V^{AN}(\lambda)$ for A>3**
2. **Improving many-body convergence**

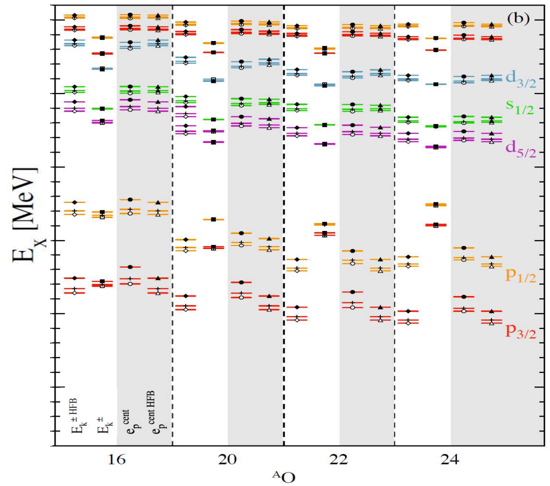


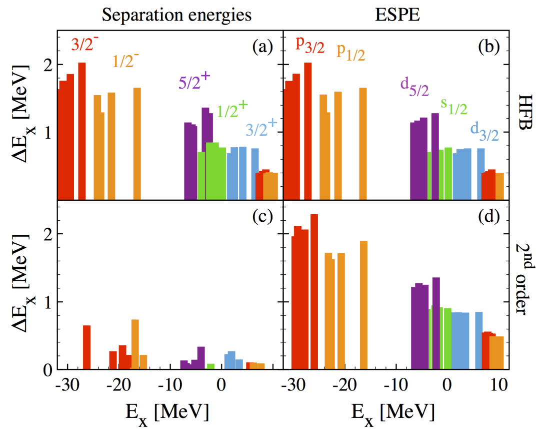


Non-observable shell structure

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

Origin: independent particle picture

Independent-particle picture

- Cornerstone of any nuclear model
- Nucleons orbit independently in

$$h = \sum_{i=1}^{N} \left(\frac{p_i^2}{2m} + V(\vec{r}_i) \right)$$

- Justified by mean free path $\sim$ 15fm
- Justified by nucleon transfer exp.

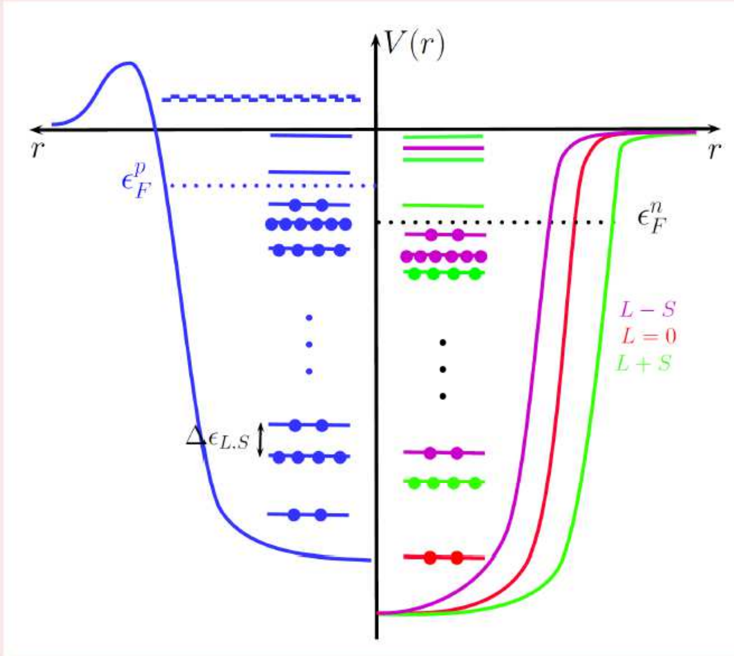
Nuclear shells

- Nucleon orbitals $\psi_\alpha = \psi_{nljm\tau}$

$$h\,\psi_{nljm\tau} = e_{nlj\tau}\,\psi_{nljm\tau}$$

- Nucleon shell-structure $e_{nlj\tau}$
- A shell is $2j+1$-fold degenerate
- Fill shells for given (N,Z)

Average one-nucleon potential $V(r_i)$



- Analogy with atomic case
- Self-created
- One for neutrons/protons
- Coulomb effect for protons
- Includes a spin-orbit component

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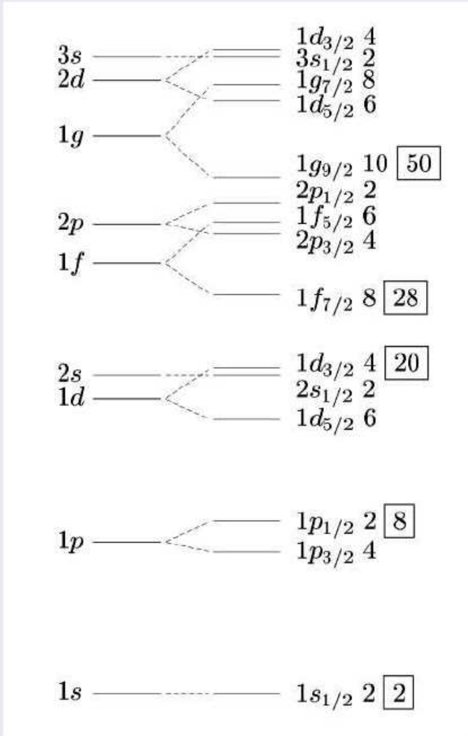
Neutron/proton shells



- Magic number = shell filled up
- (N, Z) = 2,8,20,28,50,82,126
- Spin-orbit component needed

Any reminiscence in fully interacting many-body problem?

A better one-body like picture?

Partitioning of one-nucleon separation energies

$$E_{\mu}^{+} \equiv \sum_{p} s_{\mu}^{+pp}(\lambda)\, e_{p}^{\text{cent}}(\lambda) + \sum_{pq} s_{\mu}^{+pq}(\lambda)\, \Sigma_{qp}^{\text{dyn}}(E_{\mu}^{+};\lambda)$$

Improved one-body like picture

ESPE with dominant strength not safe

$$E_{\mu}^{+} \overset{?}{\approx} e_{p}^{\text{cent}}(\lambda)$$

1. **Not good account of E^{+}_{μ} in general**
2. **Significant scale dependence**

Dominant *weighted* ESPE much superior

$$E_{\mu}^{+} \overset{?}{\approx} s_{\mu}^{+pp}(\lambda)\, e_{p}^{\text{cent}}(\lambda)$$

1. **Better account of E^{+}_{μ} in general**
2. **Reduced scale dependence**
3. **Reminds of direct cross section factorization**