Many-body correlations: the relative nature of their definition and the non-observable character of their value



Vittorio Somà CEA Saclay

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Outline

• Part I: Relative nature of many-body correlations

- Introduction: quasiparticles, correlations & many-body methods
- Examples in nuclei and nuclear matter
- Nuclear Hamiltonians & similarity renormalisation group techniques
- \circ Correlations and resolution scale

• Part II: Non-observable character of the nuclear shell structure

- \circ Single-nucleon shells \Leftrightarrow correlated nucleon dynamics
- Definition & properties of effective single-particle energies
- Scale dependence & non-observability of effective single-particle energies
- Fermi gaps & spectroscopic factors

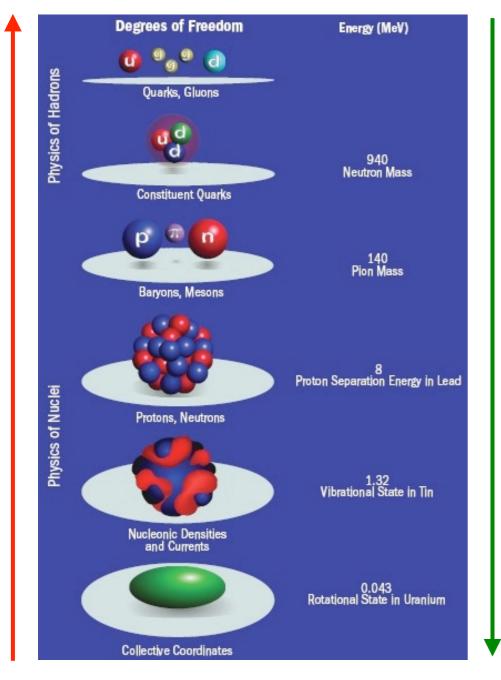
Conclusions

Part I

Relative nature of many-body correlations

Physical systems as a many-body problem

Emergent phenomena amenable to effective descriptions



- Quantum/mesoscopic system as many-body problem
- Choice of degrees of freedom

Physical system in terms of correlations between d.o.f.

- Many-body Schrödinger equation
 - \circ Exact solution for *A*=2, 3, 4
 - Approximated solution for $A \ge 5$

Accuracy/difficulty depend on correlations

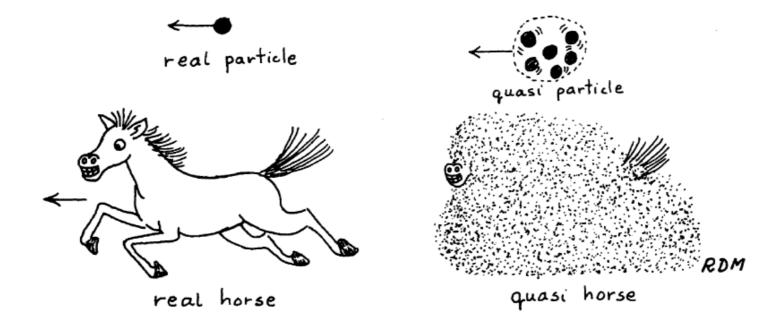
- At a given *A*, how to minimise correlations?
- When increasing *A*, how to monitor the accuracy?

Quasiparticles

● Difficulty as the number of particles increases → how to picture/model many-body correlations?
● Easy to deal with independent particles → reformulate in terms of *A* × one-body problems
● Can we change the (nature of the) chosen degrees of freedom & eliminate many-body correlations?
● Concept of (Landau) quasiparticles

Entities with modified (in-medium, renormalised, ...) properties w.r.t. the bare d.o.f.

Many-body problem of interacting particles → one-body problem of (independent) quasiparticles

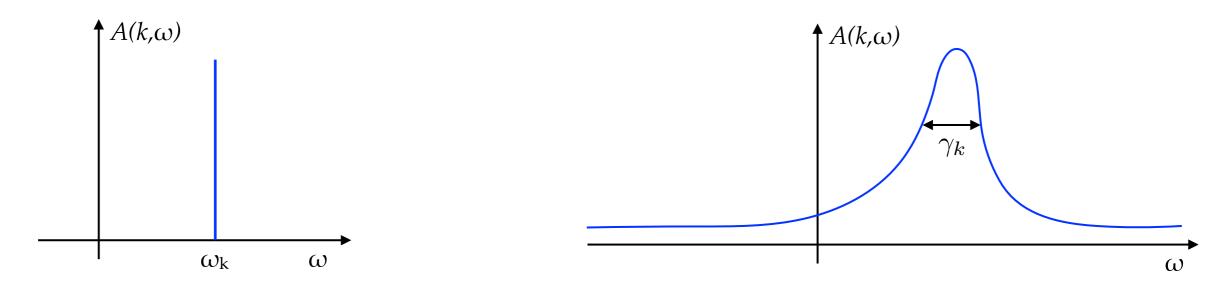


[figure from R. D. Mattuck]

Interacting quasiparticles

• In some cases, quasiparticles can be constructed explicitly

- In most cases, quasiparticles-like excitations emerge from the many-body dynamics
 - Spectral function $A(k,\omega)$ embodies quasiparticle features & many-body correlations
 - For free particles $A(k,\omega) = \delta(\omega k^2/2m)$



Infinitely-lived (=independent) quasiparticle

Decaying (=*interacting*) *quasiparticle*

● Quasiparticles with finite lifetime → departure from independent (quasi)particle picture

• Many-body correlations as residual interactions between quasiparticles

Particle-hole expansions

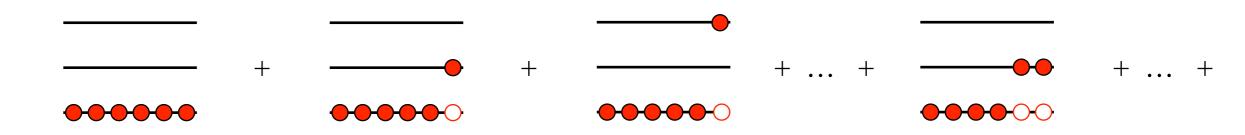
● Independent-particles as 0th-order tenet of numerous many-body methods

- \circ Perturbation theory
- \circ Density functional theory
- Nuclear shell model

• Hartree-Fock method as an optimised independent-particle description

• (Many-body) correlations: everything beyond Hartree-Fock

• Beyond-Hartree-Fock methods as expansions in particle-hole excitations

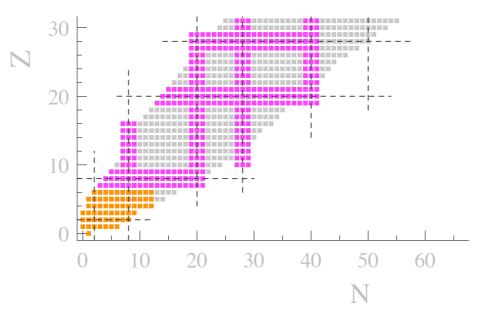


• Simplest: MBPT

- Exact (= whole expansion): Configuration interaction / No-core shell model
- Freedom to choose the interaction such that HF is the closest to the exact solution?

Different schemes for different correlations

• Methods based on particle-hole expansions face severe scaling



● Why don't include some correlation in the interaction itself? → effective interactions

- One aims at limiting the complications of ph expansions
- Interaction traditionally phenomenological, possible to derive one ab initio?

● Why don't limit ourselves to part of the Hilbert space → valence space methods

- One aims at the exact solution in the limited Hilbert space
- Interaction traditionally phenomenological, recently also ab initio

Correlations in different schemes will be different by construction

Correlations via symmetry breaking & restoration

• Correlations can be grasped by exploiting (breaking & restoration of) symmetries

 \circ For near-degenerate systems essential to expand around a symmetry-breaking reference \circ In nuclear physics: U(1) ↔ pairing correlations; SU(2) ↔ quadrupole correlations

• Can the two types be related?

Correlations included via symmetry breaking might be very hard to get via ph expansion
 And viceversa

• Can the two types be combined?

- Gorkov Green's functions [Somà, Duguet, Barbieri 2011]
- Multi-reference IM-SRG [Hergert *et al.* 2013]
- Symmetry broken & restored MBPT and CC [Duguet 2015, Duguet, Signoracci 2016]
- Many-body driven EDF [Duguet *et al.* 2015]
- Symmetry breaking & restoration + truncated CI [Ripoche et al. 2017]



Nuclear Hamiltonians

• Early Hamiltonians (60's & 70's)

 \circ Soft core

Could not reproduce nuclear saturation

• Phenomenological Hamiltonians (80's & 90's)

 \circ Hard core

• Three-body forces?

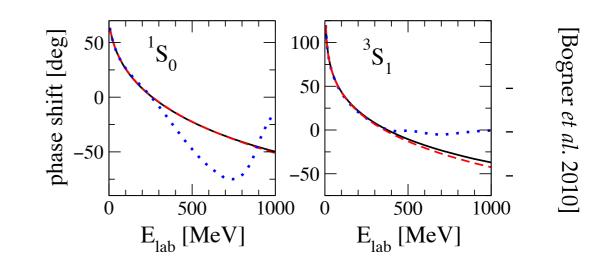
● **Chiral EFT interactions** (from 00's)

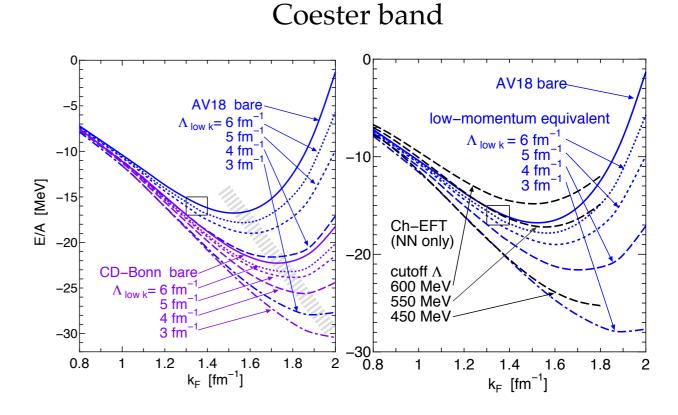
 \circ Softer core

 \circ Three-body forces consistent

• SRG techniques

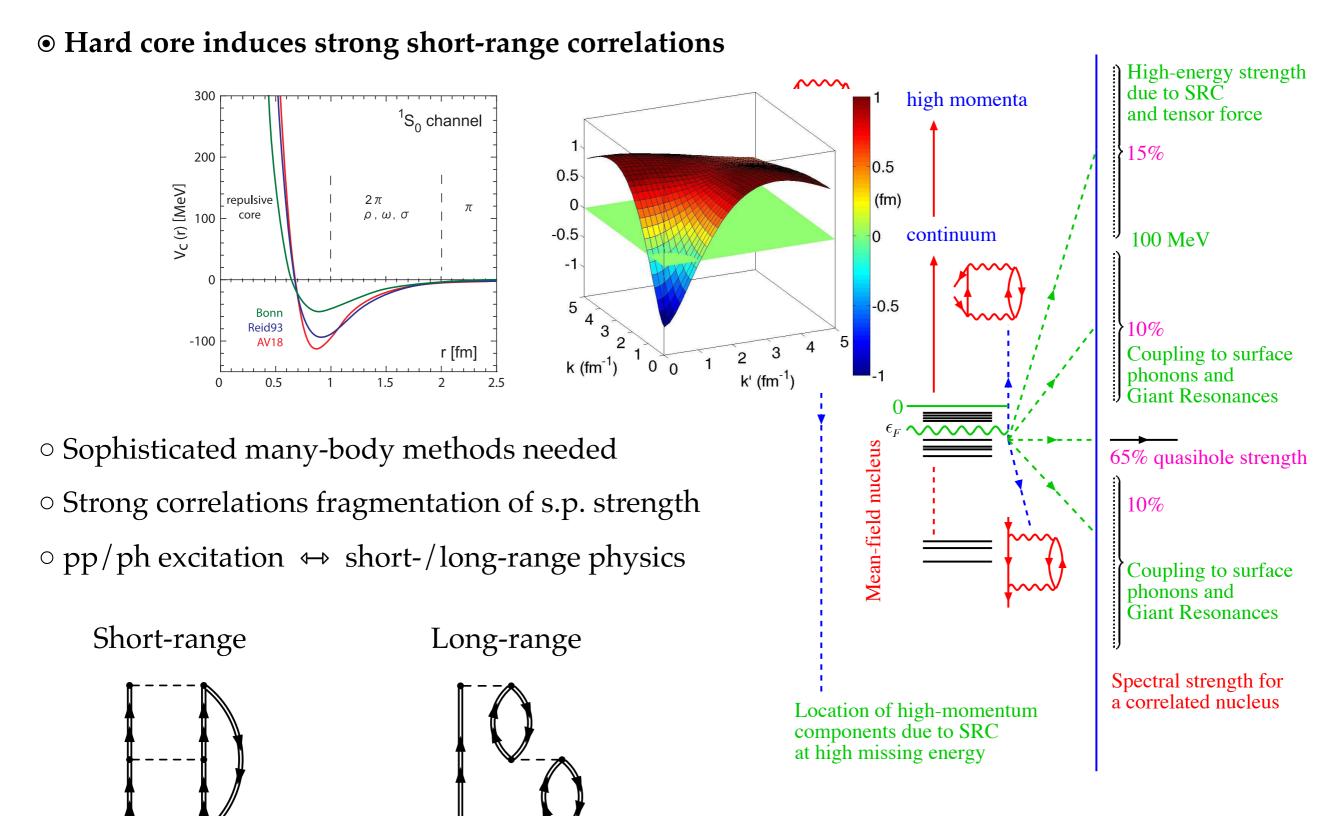
- Unitary transformation of the Hamiltonian
- Trade hard core for higher-body forces
- \circ Universality at low energy scales



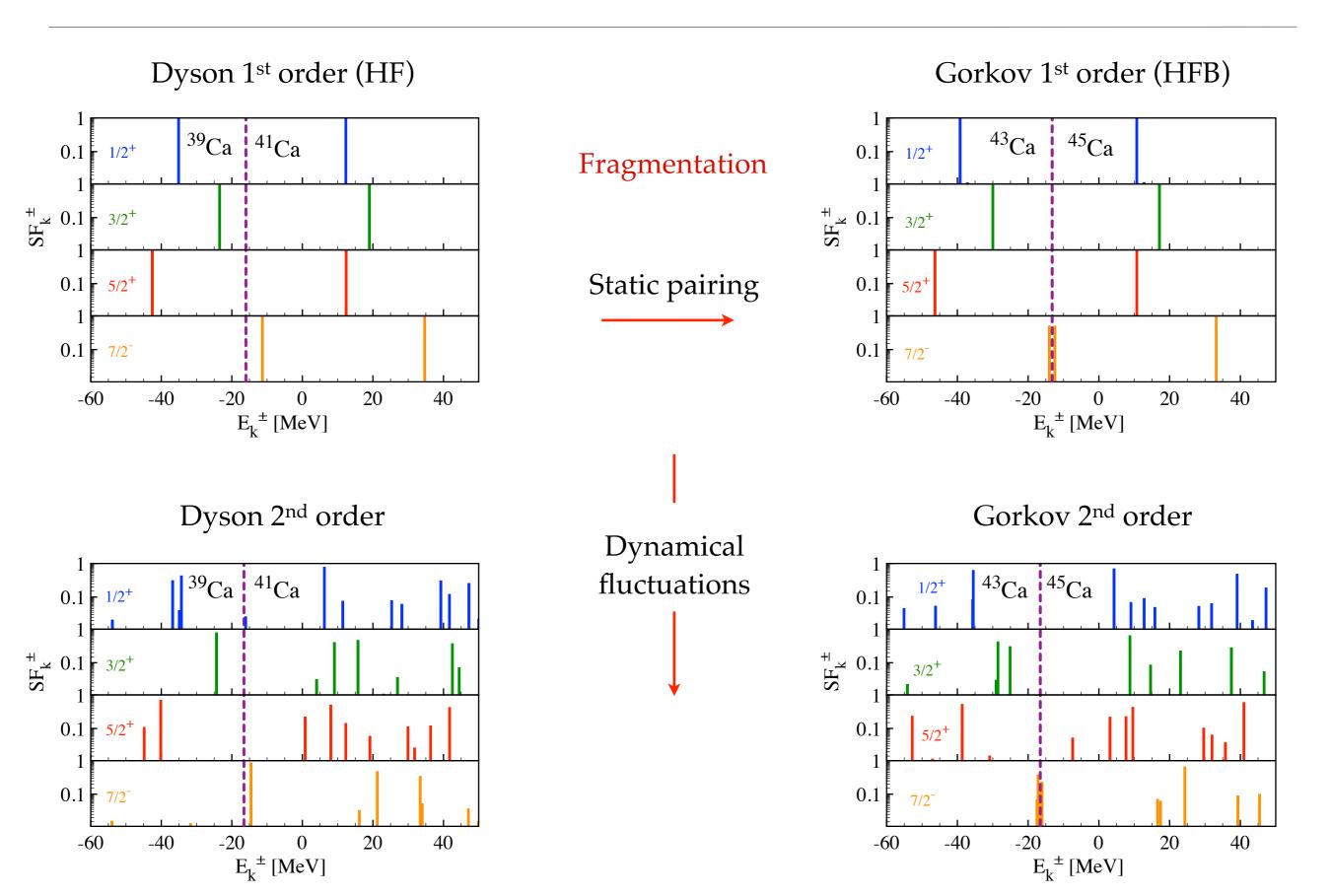


[Kohno 2015]

Long- vs short-range correlations



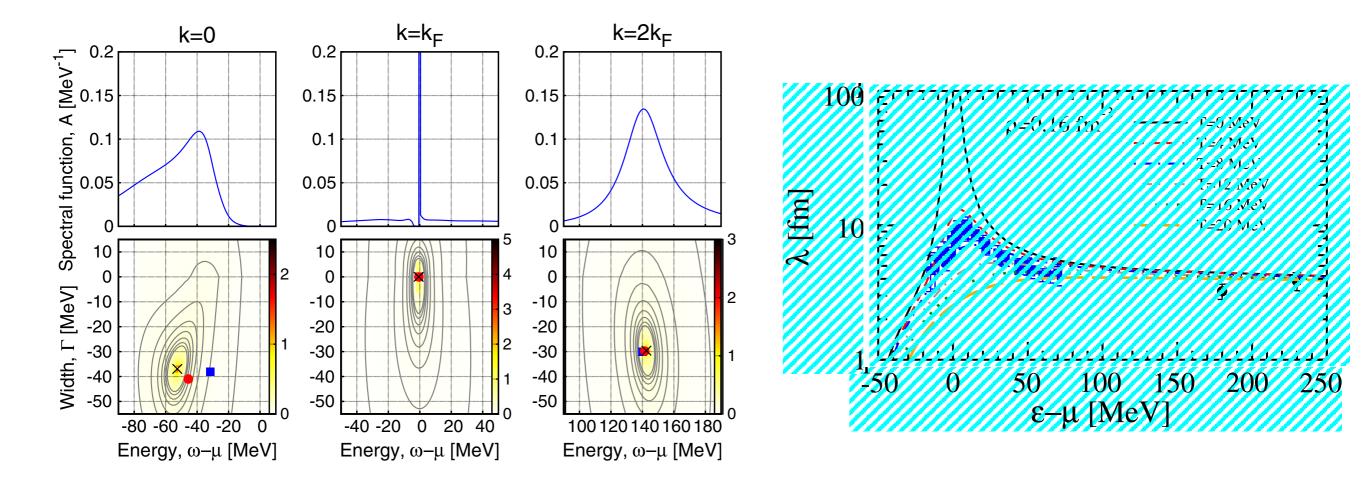
Fragmentation of single-particle strength in nuclei



Fragmentation of single-particle strength in infinite matter

• Spectral function depicts correlations

- Broad peak signals depart from
- Well-defined (long-lived) quasiparticles at the Fermi surface
- \circ Long mean free path for $E < E_{\rm F}$



Renormalisation-group techniques for nuclear forces

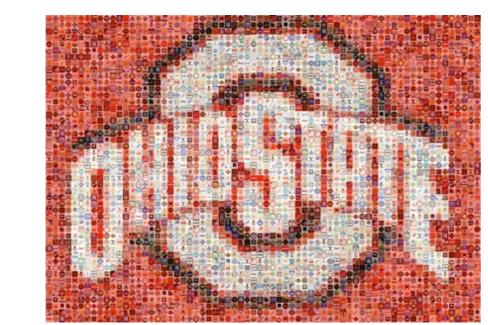
• SRC generated by couplings between low and high momenta

- Large model spaces needed to converge → applicability limited to light nuclei
- Are high momenta, i.e. high resolution, necessary to compute **low-energy observables**?



 \circ Interested in long-wavelength information

- Small-distance details irrelevant
- Change the resolution → "integrate out" unnecessary information

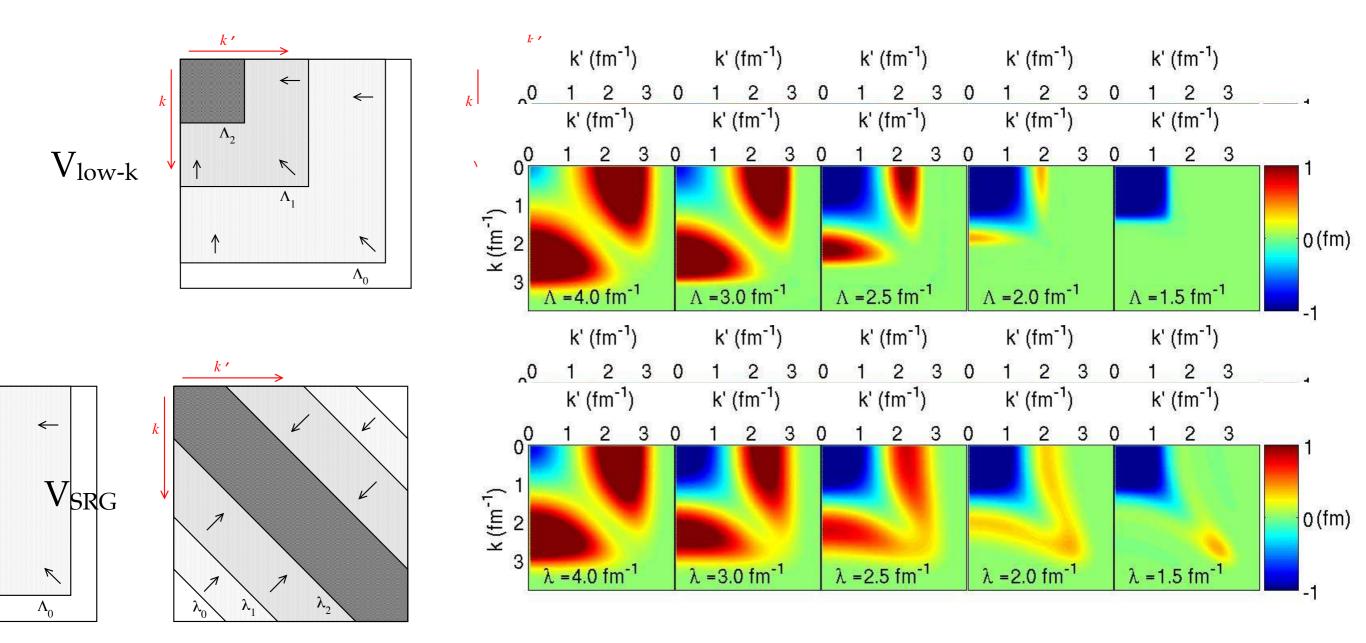




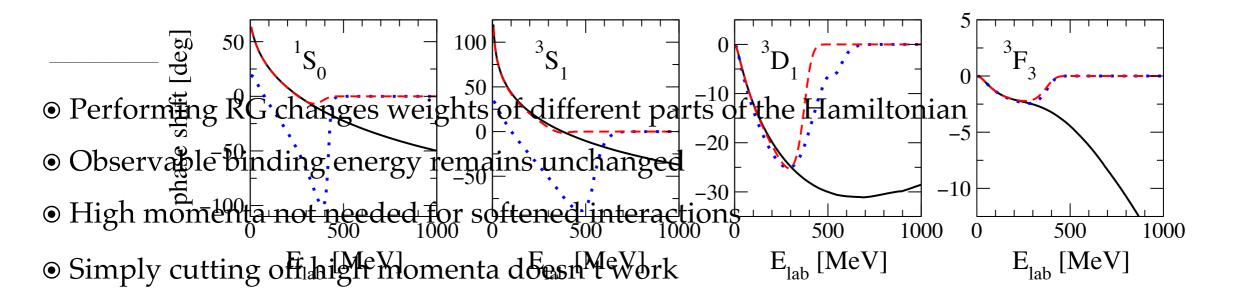
Low-momentum evolutions

• (Unitary) transformation to **change the resolution scale** of the Hamiltonian

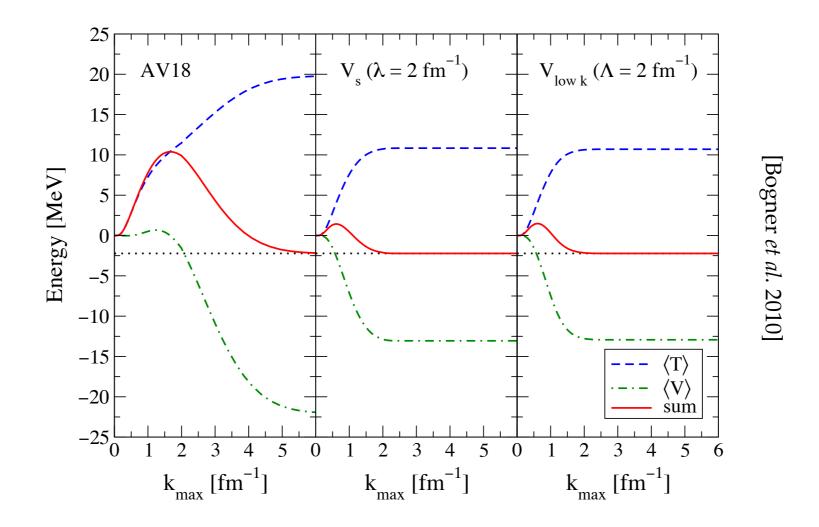
• Two main types of transformation



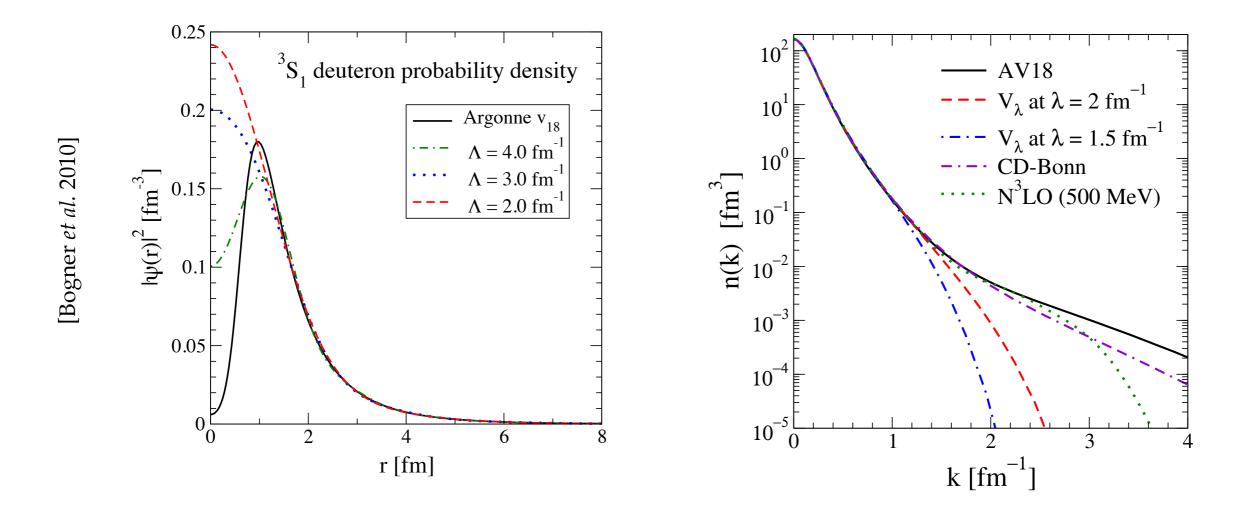
[Bogner et al. 2010]



$$E_d(k < k_{\max}) = \int_0^{k_{\max}} d\mathbf{k} \int_0^{k_{\max}} d\mathbf{k}' \,\psi_d^{\dagger}(\mathbf{k};\lambda) \left(k^2 \delta^3(\mathbf{k} - \mathbf{k}') + V_s(\mathbf{k},\mathbf{k}')\right) \psi_d(\mathbf{k}';\lambda)$$



• Short-range correlations change drastically with resolution scale

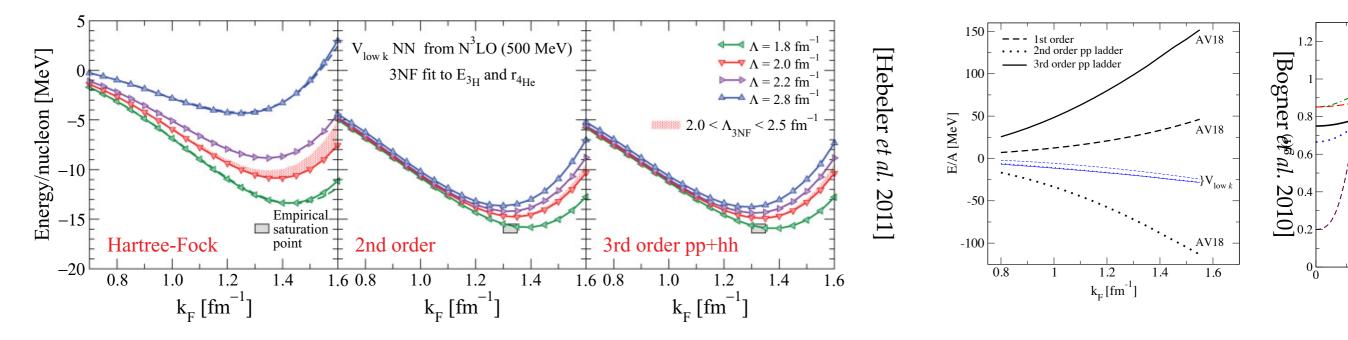


• How to explain the momentum distribution "extracted" from experiment?

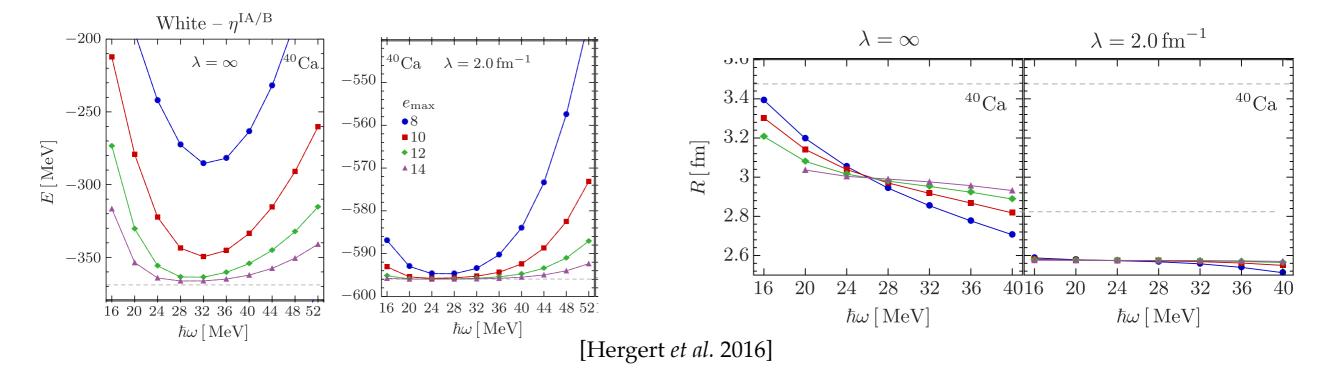
- \circ Separation between structure and reaction is scale-dependent
- Operators & currents have to evolved consistently with the Hamiltonian
- E.g. what is a one-body current at one scale, gets shifted in two-body currents at another

• Improved convergence of many-body calculations

• Smaller **model spaces** & less refined **many-body truncations** needed

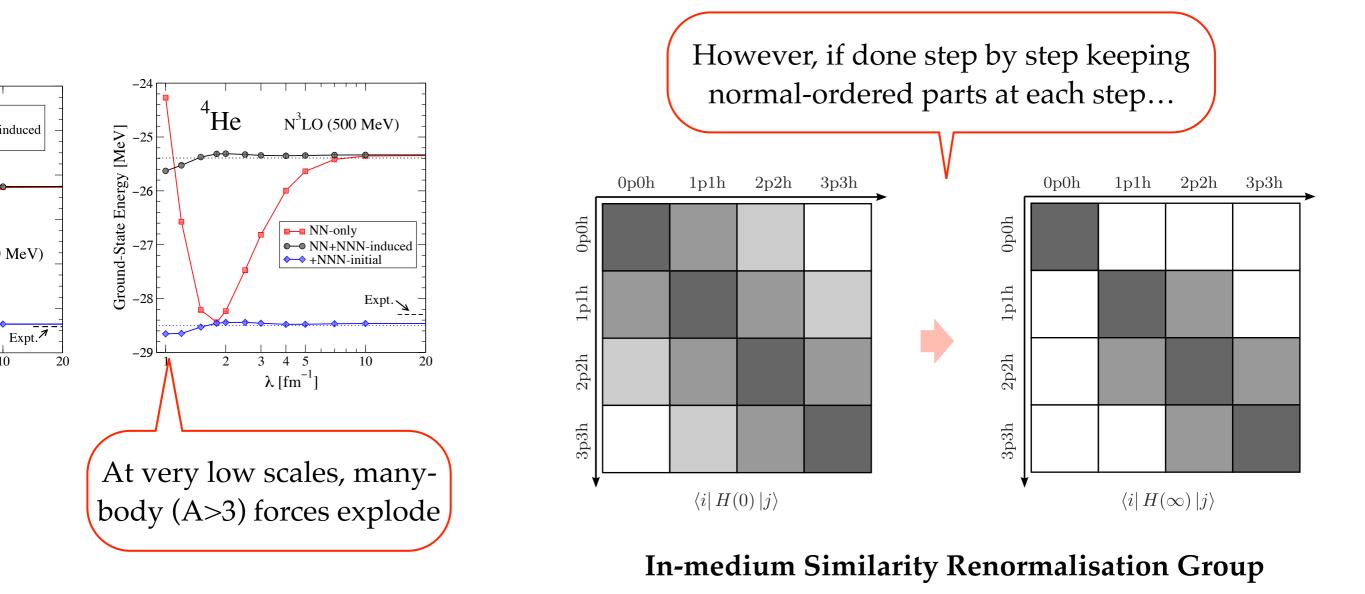


• **Drawback**: additional many-body forces generated through unitary transformation



From free space to in medium

• Why don't evolve to the point where correlations have disappeared?



• Unpractical to evolve in medium every operator we are interested in

• Combine with another many-body method (e.g. NCSM) to access wide range of observables

Part II

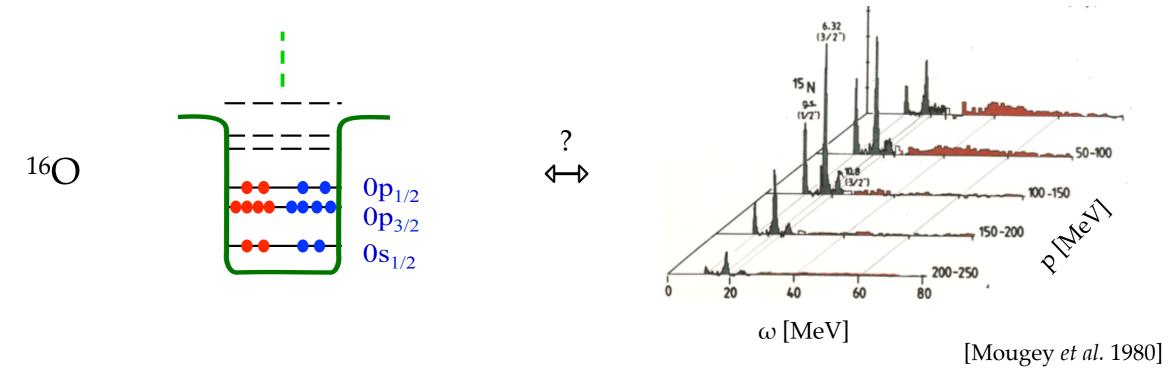
Non-observable character of the nuclear shell structure

T. Duguet, H. Hergert, J.D. Holt, V. Somà, Phys. Rev C 92 034313 (2015)

Single-nucleon shell structure

● Correlated many-body system ↔ description in terms of independent particles

• Can a one-to-one correspondence be established?



• Concept of single-nucleon shells

- \circ Basic pillar of the shell model
- \circ Provides interpretation of nuclear (low-energy) observables
- Leads to considering a single-particle spectrum (magicity, shell evolution, ...)

Useful interpretation, but which degree of reality?

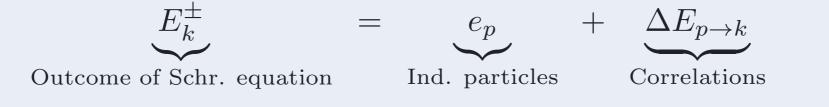
Single-nucleon shell structure

• Quantum mechanical nuclear many-body problem

○ Many-body Schrödinger equation → one-nucleon addition / removal energies

$$H|\Psi_k^{\mathcal{A}}\rangle = E_k^{\mathcal{A}}|\Psi_k^{\mathcal{A}}\rangle \qquad \qquad E_k^{\pm} \equiv \pm \left(E_k^{\mathcal{A}\pm 1} - E_0^{\mathcal{A}}\right)$$

To what extent the single-particle energy spectrum relates to low-energy observables?



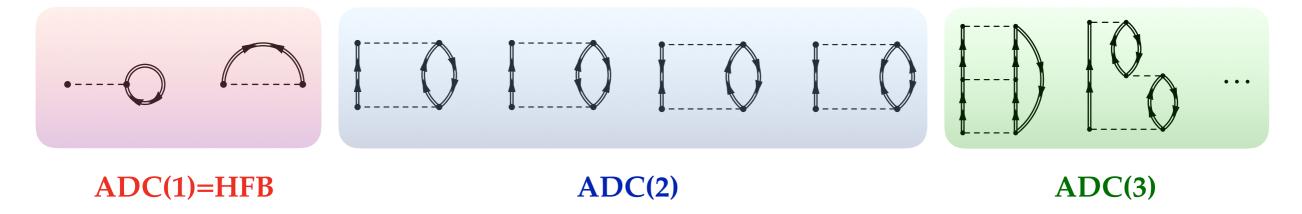
• In the following:

- Reminder of Green's function theory
- Is there a proper/unique definition of single-particle energy? → Baranger ESPEs
- Scale dependence of the above partitioning, i.e. of ESPEs
- Illustration of the scale dependence form ab initio calculations

Self-consistent Green's function approach

• Solution of the A-body Schrödinger equation $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$ achieved by

- 1) Rewriting it in terms of 1-, 2-, A-body objects $G_1=G$, G_2 , ... G_A (Green's functions)
- 2) Expanding these objects in perturbation (in practise only **G** → **one-body observables**)



• Here we employ the Algebraic Diagrammatic Construction (ADC) method

- Systematic, improvable scheme for the one-body Green's functions, truncated at order *n*
- \circ ADC(1) = Hartree-Fock(-Bogolyubov); ADC(∞) = exact solution
- At present ADC(1), ADC(2) and ADC(3) are implemented and used

● Extension to open-shell nuclei: (symmetry-breaking) Gorkov scheme

• Developed at Saclay & Surrey 2010-today [Somà, Duguet & Barbieri 2011]

Spectral representation

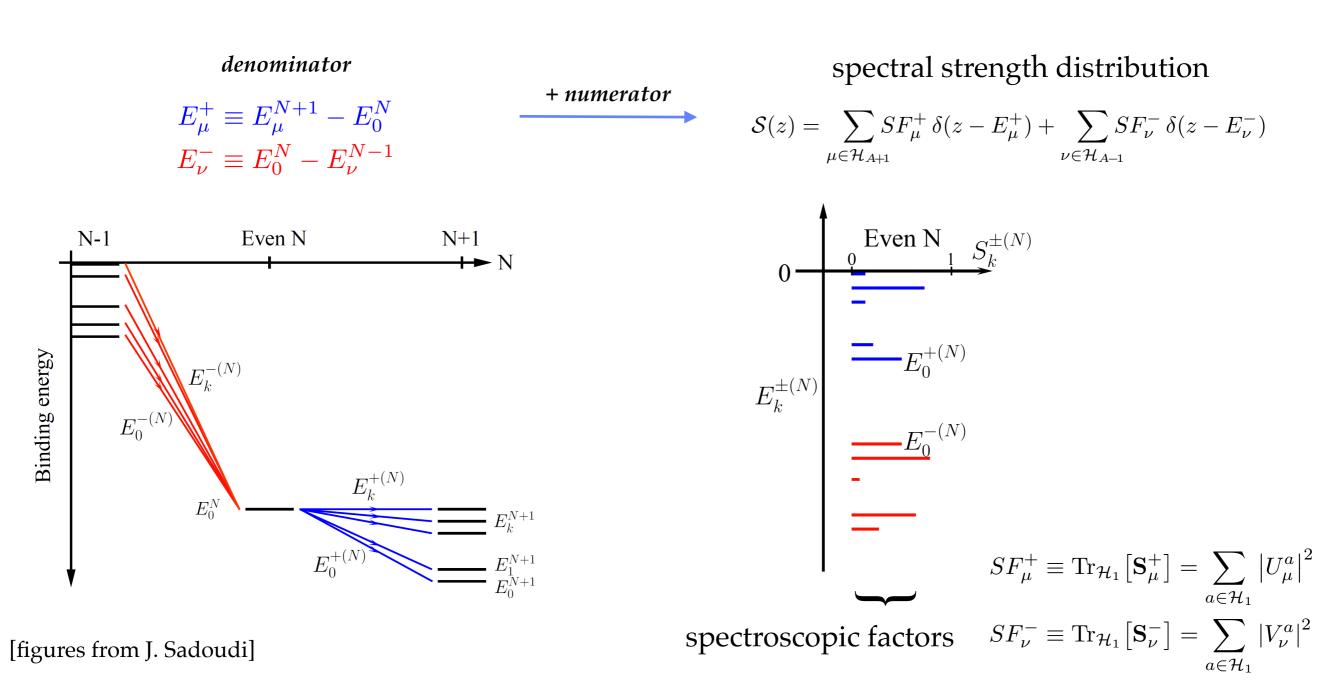
• Numerator contains spectroscopic information

$$\begin{split} G_{ab}(z) &= \sum_{\mu} \frac{\langle \Psi_{0}^{A} | a_{a} \mid \Psi_{\mu}^{A+1} \rangle \langle \Psi_{\mu}^{A+1} \mid a_{b}^{\dagger} | \Psi_{0}^{A} \rangle}{z - E_{\nu}^{+} + i\eta} + \sum_{\nu} \frac{\langle \Psi_{0}^{A} | a_{b}^{\dagger} \mid \Psi_{\nu}^{A-1} \rangle \langle \Psi_{\nu}^{A-1} \mid a_{a} | \Psi_{0}^{A} \rangle}{z - E_{\nu}^{-} - i\eta} \end{split}$$
spectroscopic amplitudes
$$\begin{split} U_{\mu}^{b} &\equiv \langle \Psi_{0}^{A} | a_{b} \mid \Psi_{\mu}^{A+1} \rangle \\ V_{\nu}^{b} &\equiv \langle \Psi_{0}^{A} | a_{b}^{\dagger} \mid \Psi_{\nu}^{A-1} \rangle \end{split}$$
spectral function
S(z) &\equiv \sum_{\mu \in \mathcal{H}_{A+1}} \mathbf{S}_{\mu}^{+} \delta(z - E_{\mu}^{+}) + \sum_{\nu \in \mathcal{H}_{A-1}} \mathbf{S}_{\nu}^{-} \delta(z - E_{\nu}^{-}) \end{aligned}
spectral strength distribution
S(z) &\equiv \operatorname{Tr}_{\mathcal{H}_{1}}[\mathbf{S}_{\nu}^{-1}] = \sum_{a \in \mathcal{H}_{1}} |U_{\mu}^{a}|^{2} \\ SF_{\nu}^{-} &\equiv \operatorname{Tr}_{\mathcal{H}_{1}}[\mathbf{S}_{\nu}^{-1}] = \sum_{a \in \mathcal{H}_{1}} |V_{\nu}^{a}|^{2} \end{aligned}

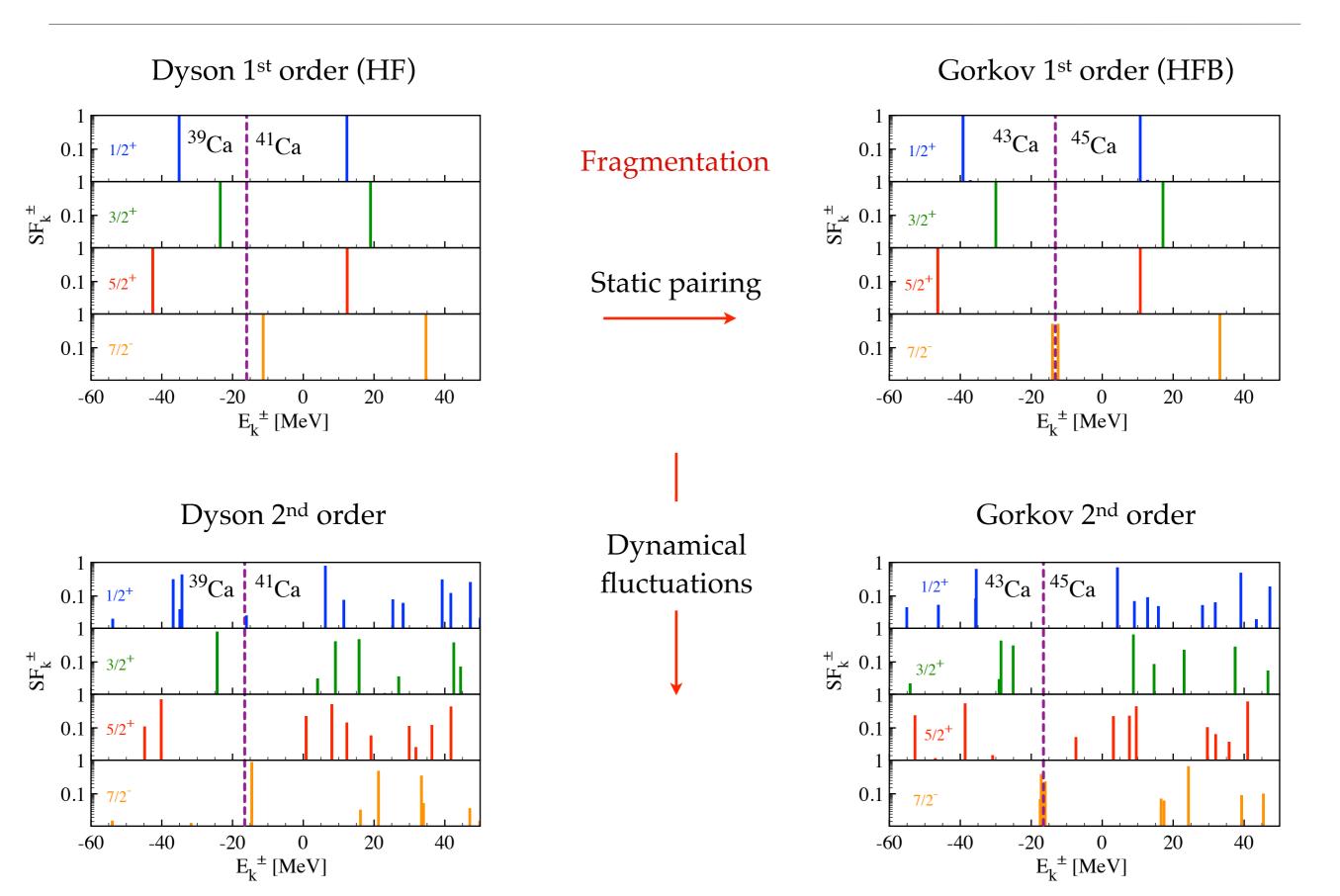
Spectral representation

• Combine numerator and denominator of Lehmann representation

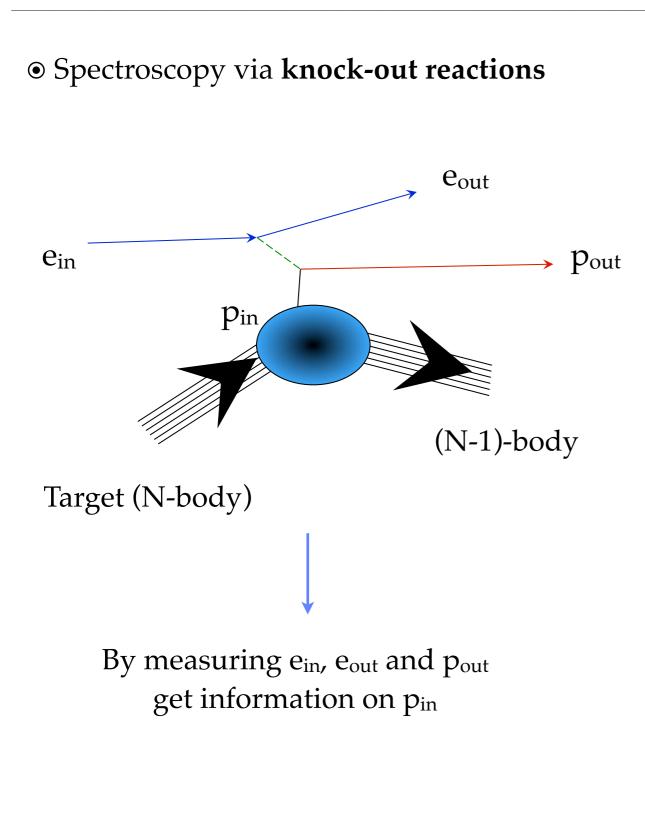
$$G_{ab}(z) = \sum_{\mu} \frac{U_a^{\mu} (U_b^{\mu})^*}{z - E_{\mu}^+ + i\eta} + \sum_{\nu} \frac{(V_a^{\nu})^* V_b^{\nu}}{z - E_{\nu}^- - i\eta}$$

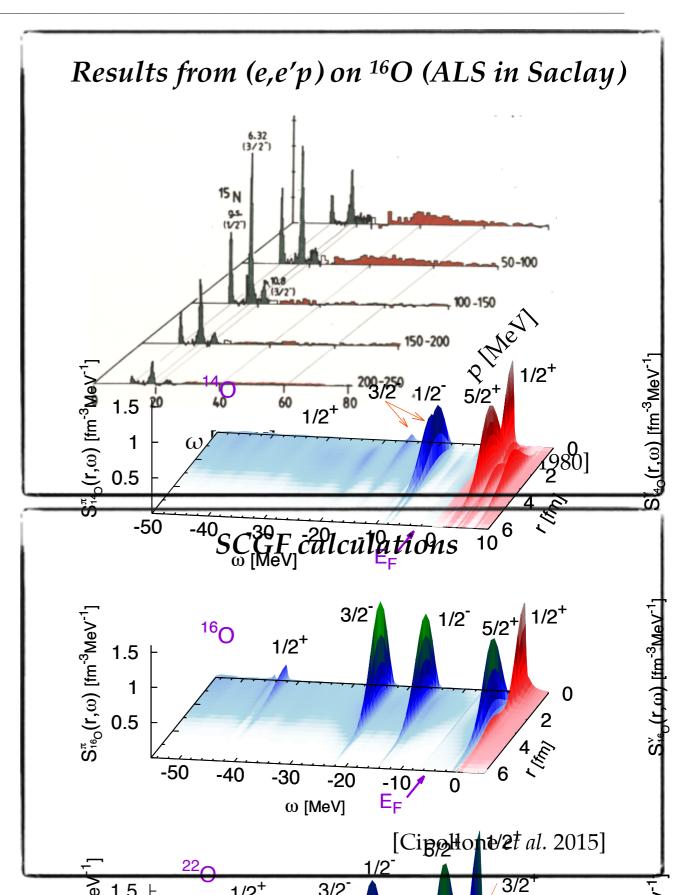


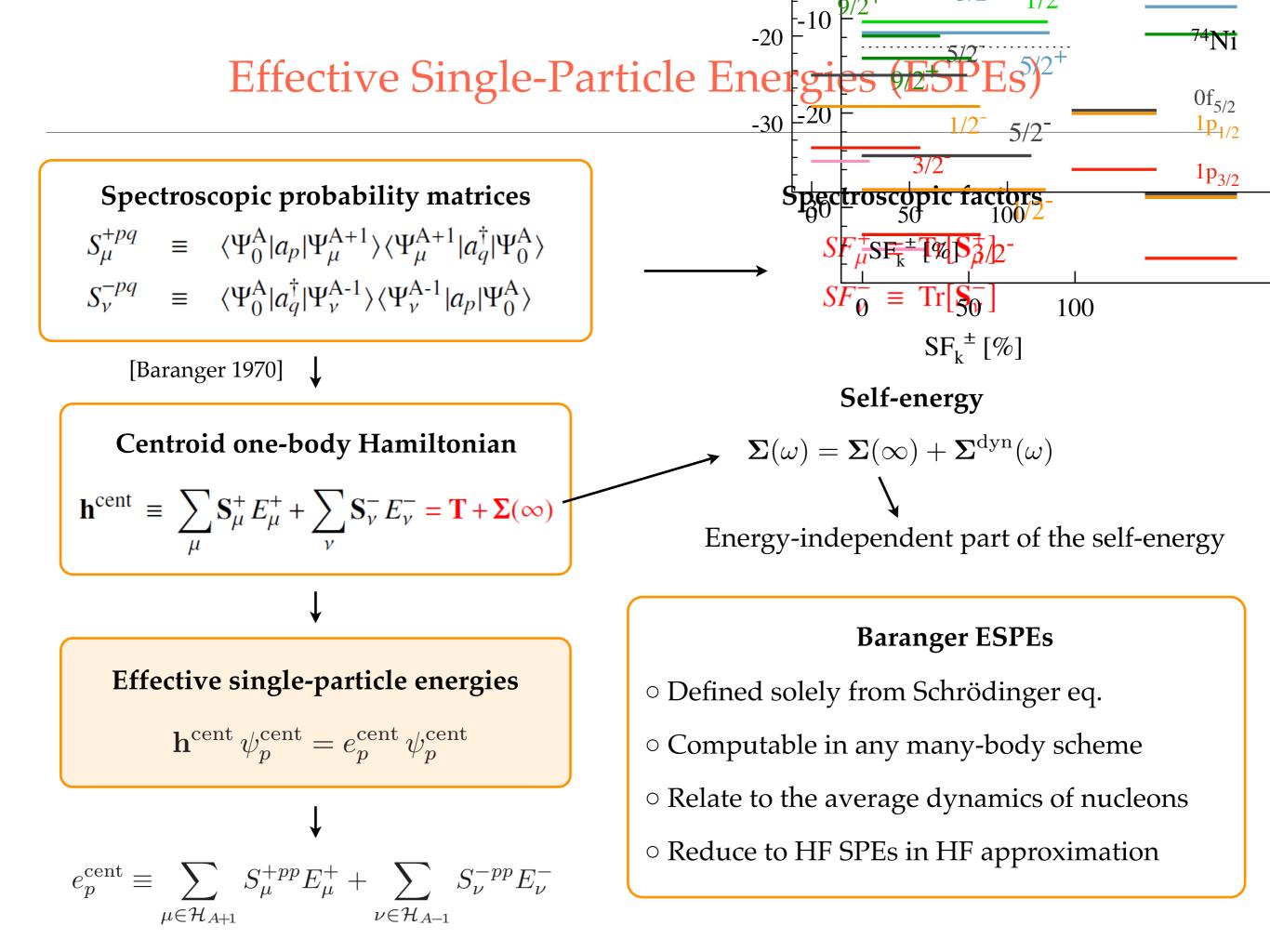
Spectral strength distribution



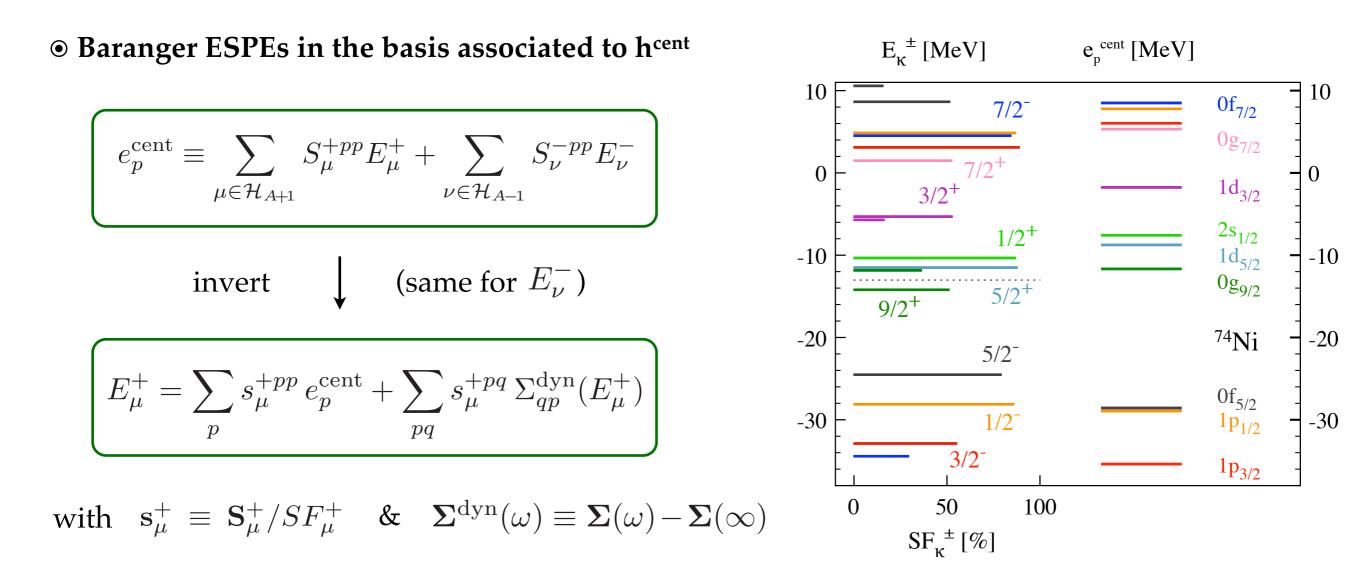
Spectral strength in experiments







Inverting ESPEs



• Rigorous partitioning into independent-particle + correlation contributions

- Exact result, no approximations so far
- A given one-nucleon addition energy does not relate to a single ESPE
- Connection between the two spectra is of matrix character

Partitioning & scale dependence

 \odot Nuclear Hamiltonian carries an intrinsic scale resolution Λ_{init}

 \odot One can further apply a unitary transformation U(λ) over Fock space

$$H(\lambda) \equiv U(\lambda)HU^{\dagger}(\lambda)$$
$$\left|\Psi_{\mu}^{A}(\lambda)\right\rangle \equiv U(\lambda)\left|\Psi_{\mu}^{A}\right\rangle$$

 $H(\lambda) \left| \Psi^A_\mu(\lambda) \right\rangle = E^A_k \left| \Psi^A_\mu(\lambda) \right\rangle$

• Any other operator transforms accordingly

$$O(\lambda) \equiv U(\lambda)OU^{\dagger}(\lambda) \equiv O^{1N}(\lambda) + O^{2N}(\lambda) + O^{3N}(\lambda) + \cdots$$

• Spectroscopic amplitudes defined at any value of λ

$$U^{p}_{\mu}(\lambda) \equiv \left\langle \Psi^{A}_{0}(\lambda) \middle| a_{p} \middle| \Psi^{A+1}_{\mu}(\lambda) \right\rangle$$
$$V^{p}_{\nu}(\lambda) \equiv \left\langle \Psi^{A}_{0}(\lambda) \middle| a^{\dagger}_{p} \middle| \Psi^{A-1}_{\nu}(\lambda) \right\rangle$$

• Generator of the transformation

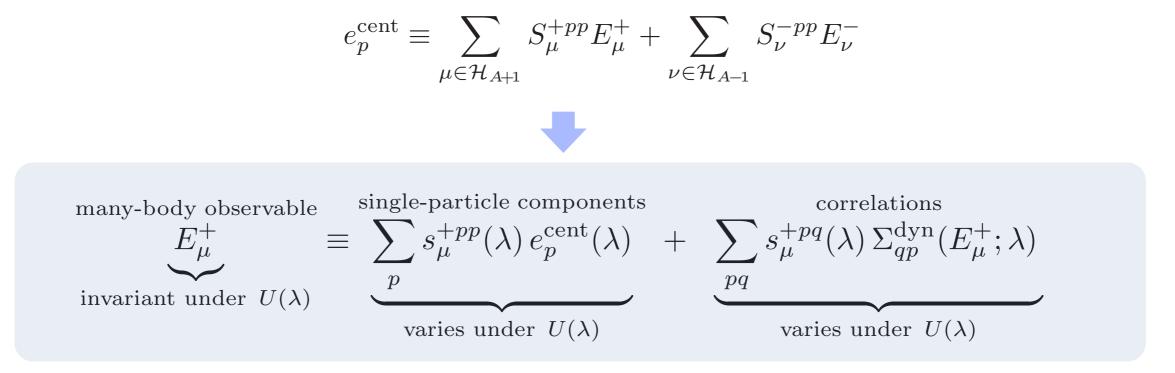
$$\eta(\lambda) \equiv \frac{dU(\lambda)}{d\lambda} U^{\dagger}(\lambda)$$

Partitioning & scale dependence

• Spectroscopic probabilities / factors are **scale-dependent**

$$\frac{d}{d\lambda}V_{\nu}^{p}(\lambda) = -\left\langle\Psi_{\nu}^{A-1}(\lambda)\big|[\eta(\lambda),a_{p}]\big|\Psi_{0}^{A}(\lambda)\right\rangle^{*}$$
$$\frac{d}{d\lambda}U_{\mu}^{p}(\lambda) = -\left\langle\Psi_{\mu}^{A+1}(\lambda)\big|[\eta(\lambda),a_{p}^{\dagger}]\big|\Psi_{0}^{A}(\lambda)\right\rangle^{*}$$

• ESPEs acquire scale dependence via spectroscopic probabilities

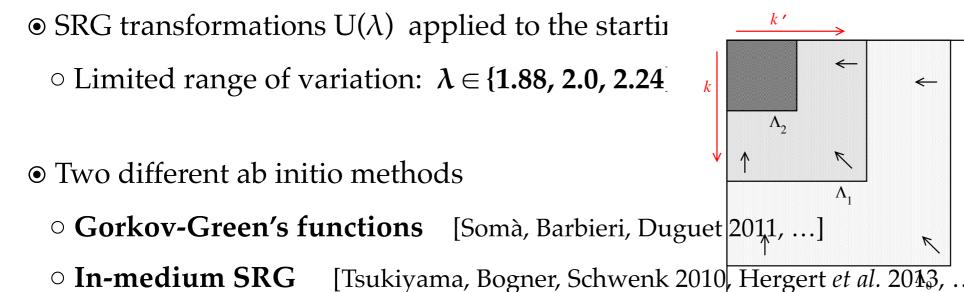


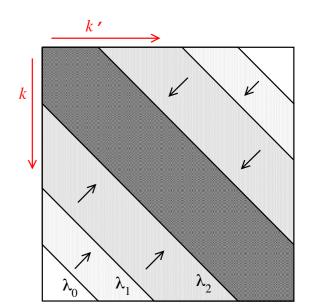
 \circ A convenient choice of λ maximises the ESPE component

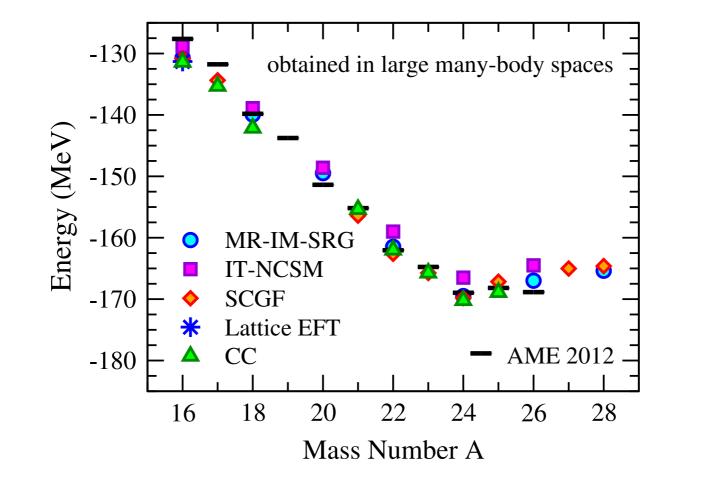
 \circ However, correlations with observables are not absolute

 \circ Scale must be fixed/specified prior to theoretical/experimental comparisons

SRG transformation & ab initio calculations









Breaking of unitarity

• Unitarity artificially broken

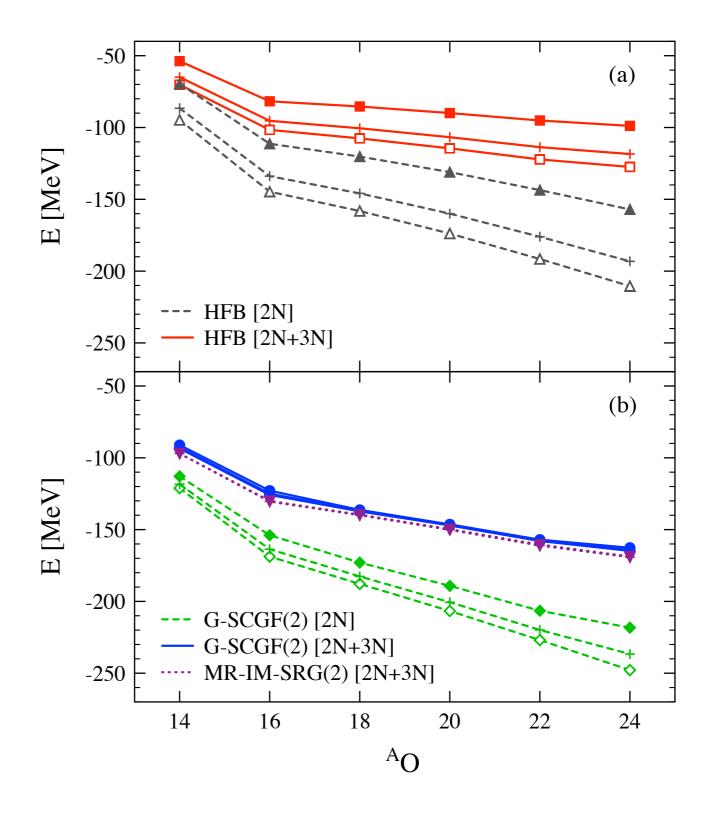
- Omission of *A*-body operators with *A*>3
- \circ Many-body truncations

• Breaking can be estimated

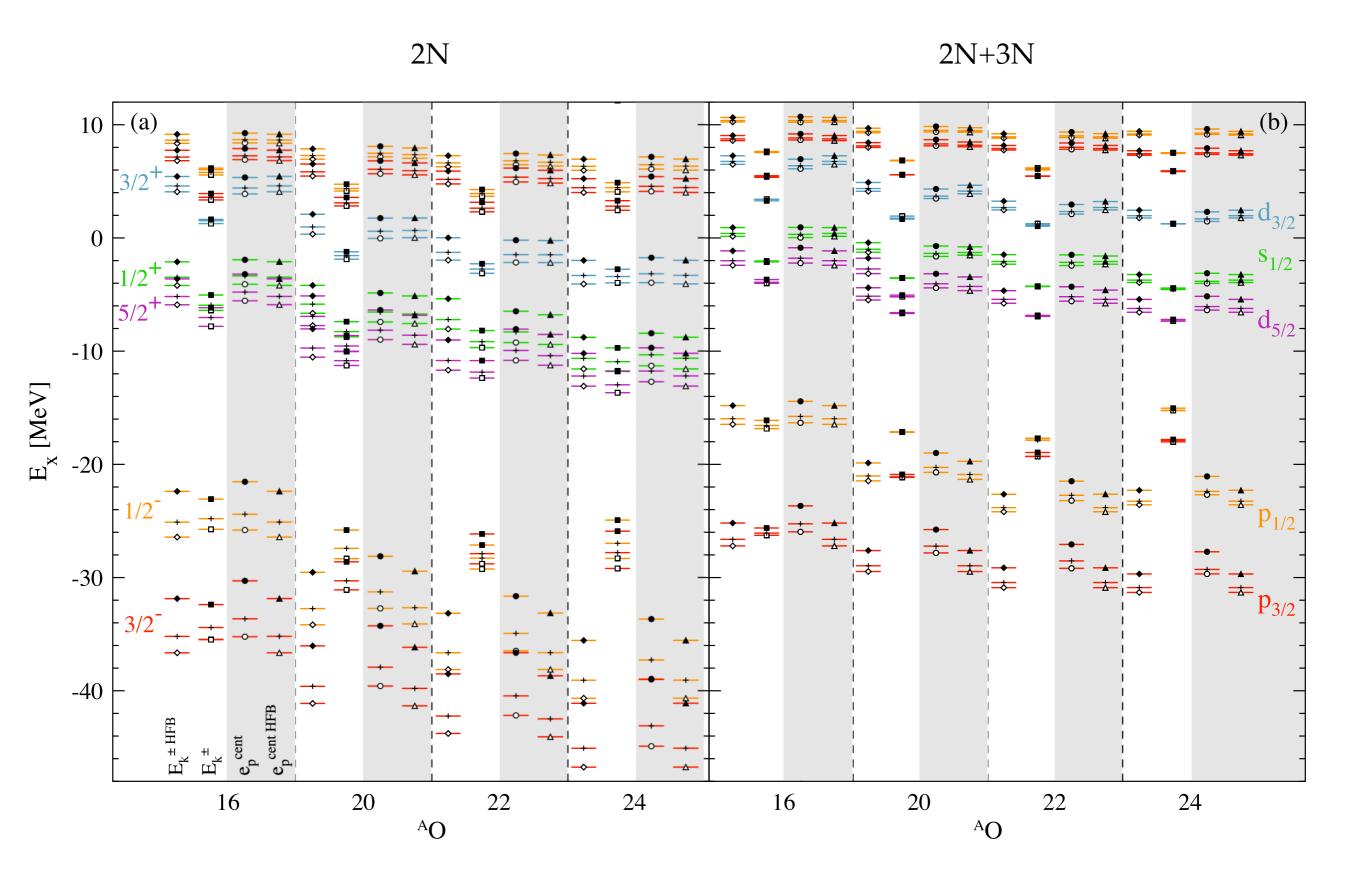
Omitting 3-body operatorsDegrading the many-body truncation

• Breaking for total energy

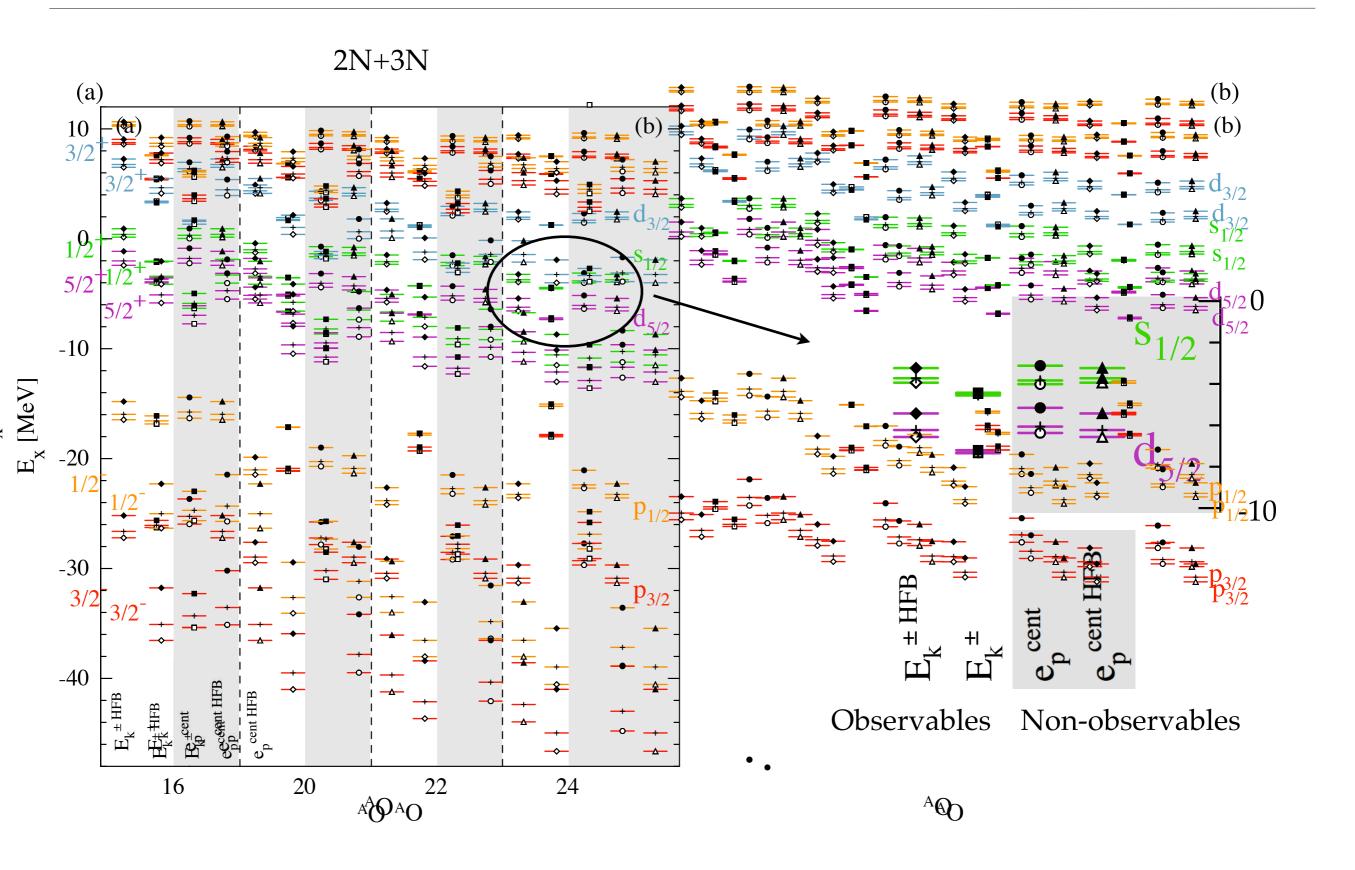
- Around 1 MeV for GGF
- \circ Around 100 keV for IM-SRG



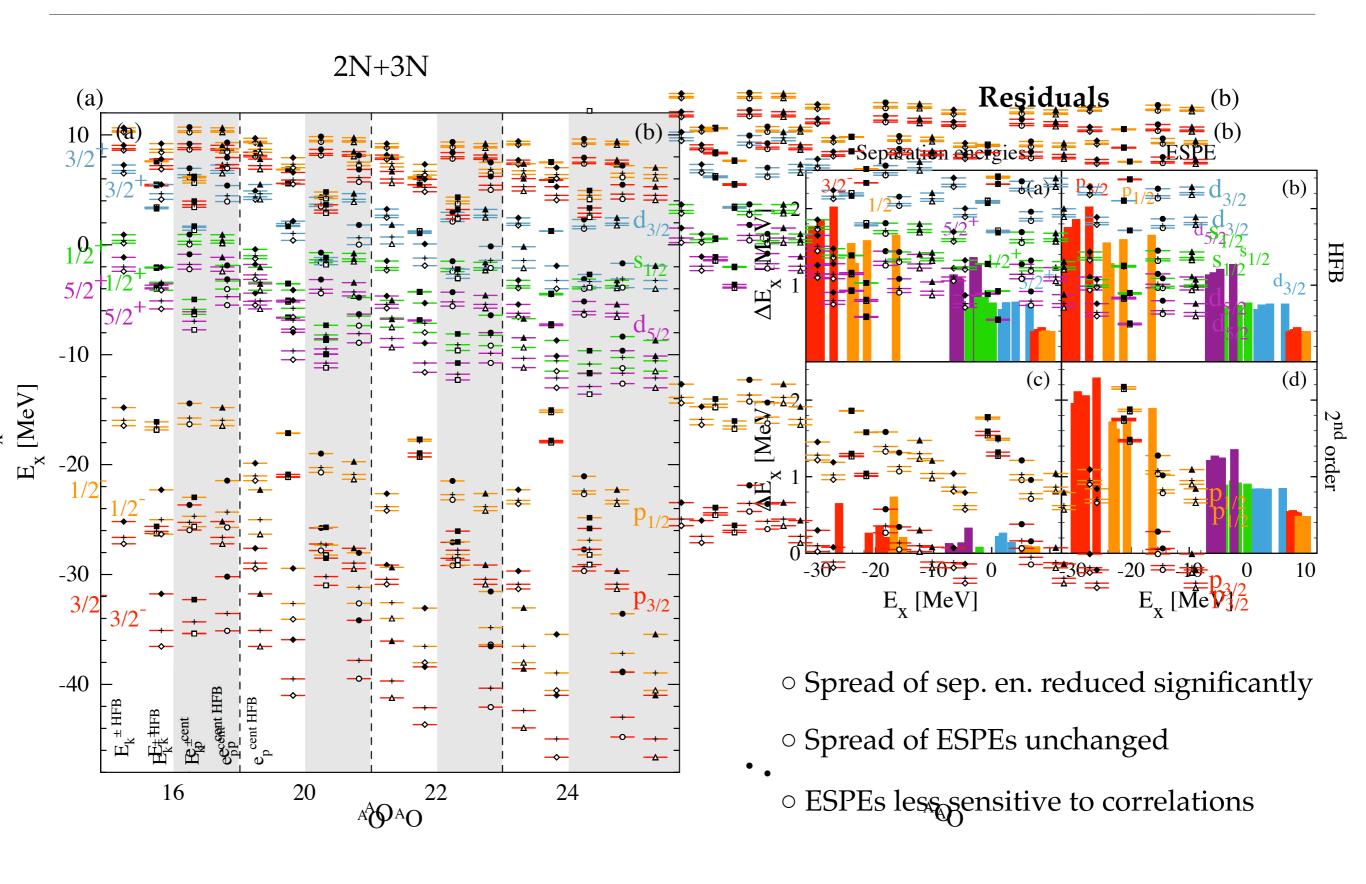
Scale (in)dependence of separation energies & ESPEs



Scale (in)dependence of separation energies & ESPEs



Scale (in)dependence of separation energies & ESPEs

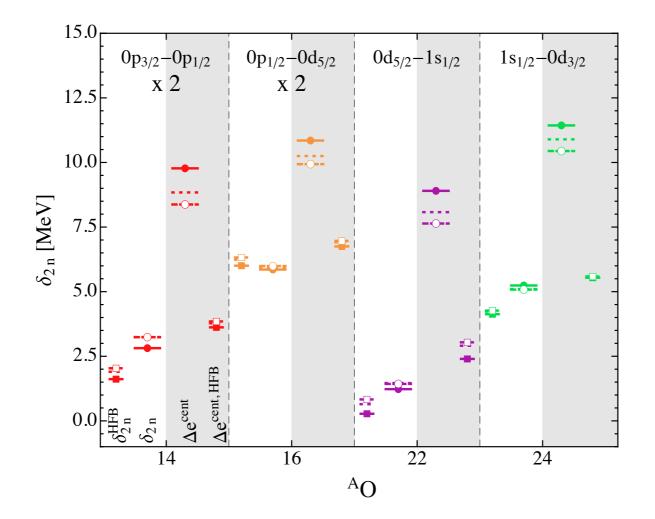


Shell gaps

• Gaps across the Fermi energy (equal in the HF limit)

- (Observable) two-neutron shell gap $\delta_{2n}(N,Z) \equiv \frac{1}{2} \left[E(N+2,Z) 2E(N,Z) + E(N-2,Z) \right]$
- (Non-observable) ESPE Fermi gap

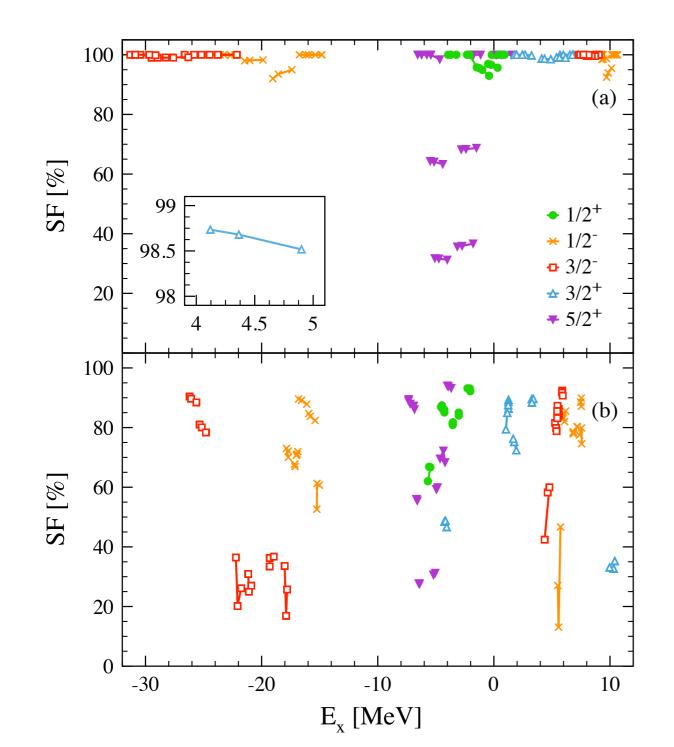
 $\Delta e_{\rm F}^{\rm cent}(N,Z) \equiv e_p^{\rm cent}(N,Z) - e_h^{\rm cent}(N,Z)$

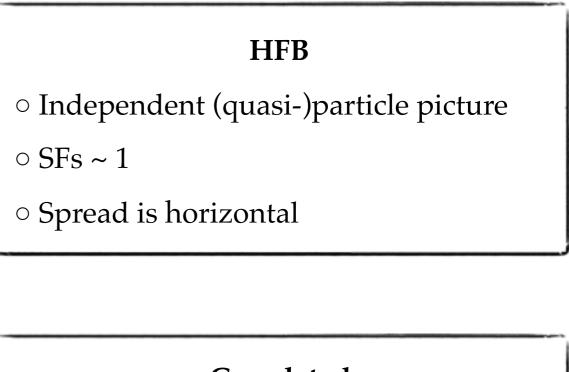


• HFB level: ESPE & 2N gaps similar, the former well captures the latter
 • Correlated calculation: scale dependence of ESPE gaps is systematically large

● Compilation of SF for one-neutron addition/removal on ¹⁴⁻²⁴O

○ Limited running with $\lambda \in \{1.88, 2.0, 2.24\}$ fm⁻¹ !





Correlated

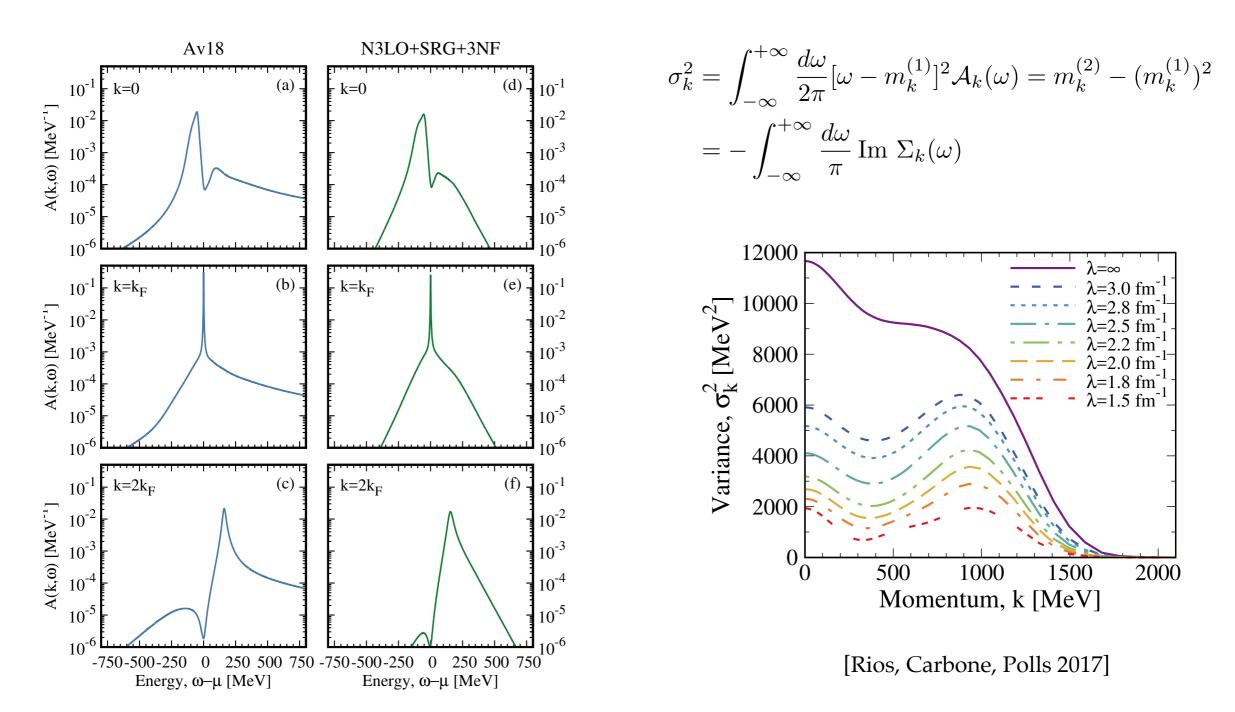
- \circ Horizontal spread minimised
- Spectroscopic strength now fragmented
- Some scale dependence of SFs appears

SRG & correlations in infinite matter

• Larger range of scales can be explored in infinite nuclear matter

 \circ Momentum tails in spectral function depend on the interaction

• Variance depicts amount of correlations



Summary

• Part I

• Correlations are scheme and scale dependent

- What balance between different ways of accounting for correlations?
- Similarity renormalisation group as a knob for (short-range) correlations

• Part II

- **Non-observability of shell structure** formally revisited
- Ab initio calculations corroborate formal analysis
- Correlations between observables & shell structure **depend on the resolution scale**
- Scale / scheme dependence should be explicit & consistent

• Perspectives

- **Quantification of scale dependence** interesting from a pragmatic point of view
- Focus should be on **consistency** to combine structure & reactions