Gorkov-Green's function theory for mid-mass nuclei

Vittorio Somà
CEA Saclay

Contents:

1. Progress & status of GGF theory

   - ♦ VS, Cipollone, Barbieri, Navrátil, Duguet, PRC 89 061301 (2014)
   - ♦ Papuga, VS, *et al.* PRC 90 034321 (2014)
   - ♦ VS, Barbieri, Cipollone, Duguet, Navrátil, *in preparation*

2. Non-observability of shell structure

   - ♦ Duguet, Hergert, Holt, VS, arXiv:1411.1237

TRIUMF
19 February 2015

Ab initio *open-shell* nuclei

✪ **Impressive progress in ab initio calculations over last few years**

- ➟ New models of nuclear interactions available (χ-EFT based)
- ➟ New techniques available (e.g. extension to open-shells, lattice, reactions)
- ➟ Thorough error assessment on the way

✪ **Self-consistent Green's functions**

- ➟ Many-body truncation in the self-energy expansion (cf. CC, IM-SRG, ...)
- ➟ Access to $A\pm1$ systems via spectral function
- ➟ Natural connection to scattering (e.g. optical potentials)

✪ **Gorkov scheme**

- ➟ Goes beyond standard expansion schemes limited to doubly closed-shell
  - ○ Formulate the expansion scheme around a Bogoliubov vacuum
  - ○ Single-reference method (cf. MR in quantum chemistry or IM-SRG)
  - ○ Exploit breaking (and restoration) of U(1) symmetry

Gorkov framework

✪ Expand around an auxiliary many-body state

$$|\Psi_0\rangle \equiv \sum_A^{\text{even}} c_A \, |\psi_0^A\rangle$$

Breaks particle-number symmetry

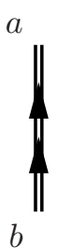
➟ Introduce a "grand-canonical" potential $\Omega = H - \mu A$

➟ $|\Psi_0\rangle$ minimizes $\Omega_0 = \langle\Psi_0|\Omega|\Psi_0\rangle$ under the constraint $A = \langle\Psi_0|A|\Psi_0\rangle$

➟ Observables of the A-body system $\Omega_0 = \sum_{A'} |c_{A'}|^2 \, \Omega_0^{A'} \approx E_0^A - \mu A$

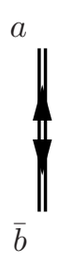
set of 4 propagators

$$i\,G_{ab}^{11}(t,t') \equiv \langle\Psi_0|T\left\{a_a(t)a_b^\dagger(t')\right\}|\Psi_0\rangle \equiv$$



$$i\,G_{ab}^{21}(t,t') \equiv \langle\Psi_0|T\left\{\bar{a}_a^\dagger(t)a_b^\dagger(t')\right\}|\Psi_0\rangle \equiv$$

$$i\,G_{ab}^{12}(t,t') \equiv \langle\Psi_0|T\left\{a_a(t)\bar{a}_b(t')\right\}|\Psi_0\rangle \equiv$$



$$i\,G_{ab}^{22}(t,t') \equiv \langle\Psi_0|T\left\{\bar{a}_a^\dagger(t)\bar{a}_b(t')\right\}|\Psi_0\rangle \equiv$$

[Gorkov 1958]

Gorkov equation & self-energy expansion

Many-body Schrödinger equation

$$H\Psi = E\Psi$$

Dyson / Gorkov equation

$$\mathbf{G}_{ab}(\omega) = \mathbf{G}^{(0)}_{ab}(\omega) + \sum_{cd} \mathbf{G}^{(0)}_{ac}(\omega)\, \boldsymbol{\Sigma}^{\star}_{cd}(\omega)\, \mathbf{G}_{db}(\omega)$$

Systematic expansion

➟ up to 2nd order implemented

➟ 3rd order on the way

Energy *dependent* eigenvalue problem

$$\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & -t_{ab} + \mu_{ab} + \Sigma^{22}_{ab}(\omega) \end{pmatrix}\Bigg|_{\omega_k} \begin{pmatrix} \mathcal{U}^k_b \\ \mathcal{V}^k_b \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k_a \\ \mathcal{V}^k_a \end{pmatrix}$$

Energy *independent* eigenvalue problem

$$\begin{pmatrix} T - \mu + \Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^\dagger \\ \tilde{h}^\dagger & -T + \mu - \Lambda & -\mathcal{D}^\dagger & \mathcal{C} \\ \mathcal{C}^\dagger & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^\dagger & 0 & -E \end{pmatrix} \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix}$$

Gorkov equation & self-energy expansion

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Single-particle propagator (Green's function) gives access to

- all one-body observables of the A system
- the total energy of the A system via Koltun's sumrule

$$\langle \hat{H} \rangle = E_0 = \sum_{ab} \int \frac{d\omega}{2\pi}\, [t_{ab} + \omega\, \delta_{ab}]\; G_{ab}(\omega)$$

Inside the Green's function

✪ Separation energy spectrum

$$G^{11}_{ab}(\omega) = \sum_k \left\{ \frac{\mathcal{U}^k_a \, \mathcal{U}^{k*}_b}{\omega - \omega_k + i\eta} + \frac{\bar{\mathcal{V}}^{k*}_a \, \bar{\mathcal{V}}^k_b}{\omega + \omega_k - i\eta} \right\}$$

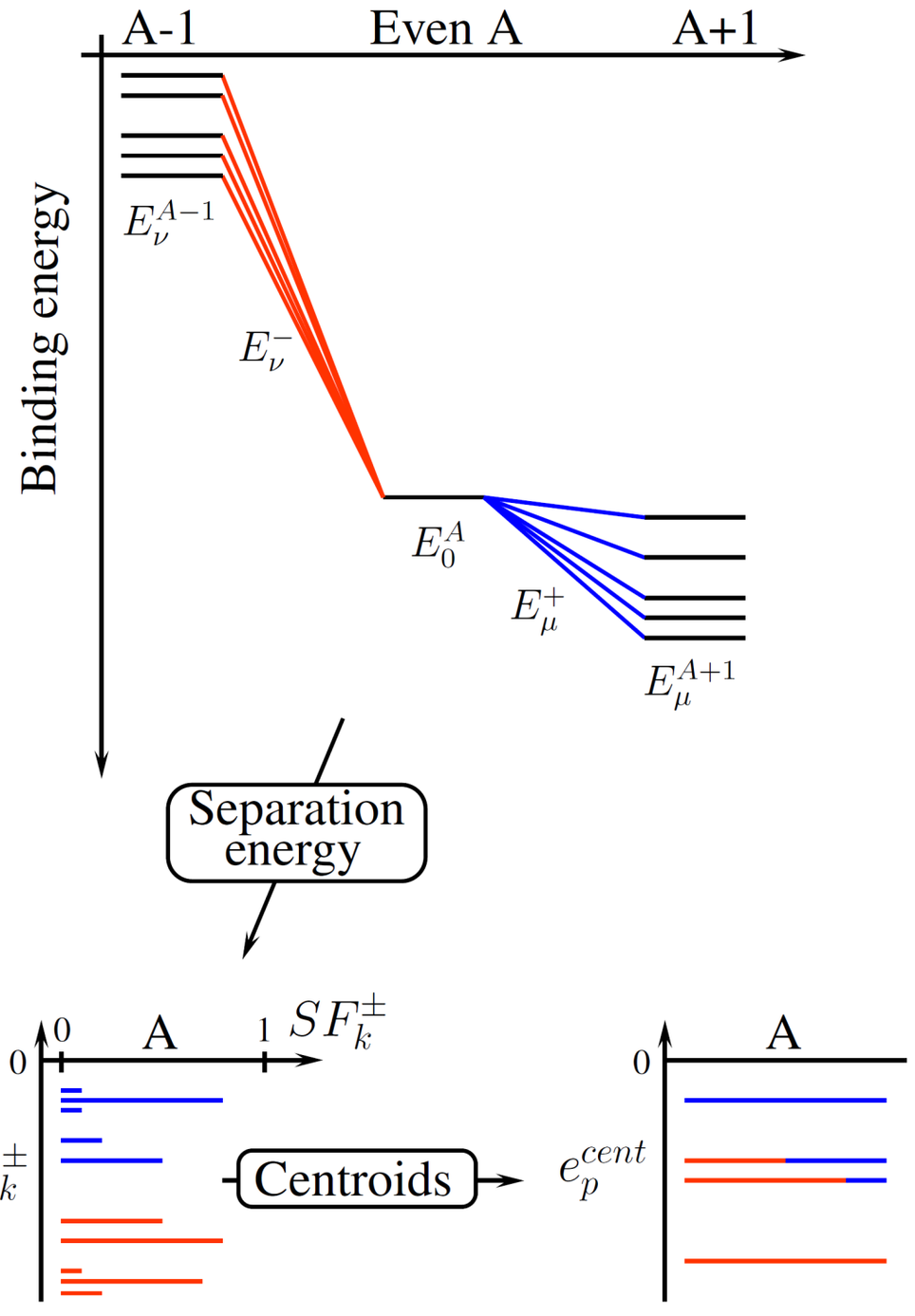
Lehmann representation

where
$$\begin{cases} \mathcal{U}^{k*}_a \equiv \langle \Psi_k | a^\dagger_a | \Psi_0 \rangle \\ \mathcal{V}^{k*}_a \equiv \langle \Psi_k | \bar{a}_a | \Psi_0 \rangle \end{cases}$$

and
$$\begin{cases} E^{+\,(A)}_k \equiv E^{A+1}_k - E^A_0 \equiv \mu + \omega_k \\ E^{-\,(A)}_k \equiv E^A_0 - E^{A-1}_k \equiv \mu - \omega_k \end{cases}$$

✪ Spectroscopic factors

$$SF^+_k \equiv \sum_{a \in \mathcal{H}_1} \left| \langle \psi_k | a^\dagger_a | \psi_0 \rangle \right|^2 = \sum_{a \in \mathcal{H}_1} \left| \mathcal{U}^k_a \right|^2$$
$$SF^-_k \equiv \sum_{a \in \mathcal{H}_1} \left| \langle \psi_k | a_a | \psi_0 \rangle \right|^2 = \sum_{a \in \mathcal{H}_1} \left| \mathcal{V}^k_a \right|^2$$



[figure from J. Sadoudi]

Setup

✪ NN & 3N chiral interactions (N^3LO 500 MeV & N^2LO 400 MeV)

SRG-evolved to 2.0 fm^{-1} [Entem and Machleidt 2003, Navrátil 2007, Roth *et al*. 2012]

✪ H.O. basis of 14 major shells; $E_{3max} = 16$

✪ Three-body forces contracted with fully correlated density matrix to obtain one- and two-body effective operators

➟ Generalisation of normal ordering

➟ Galitskii-Koltun sum rule modified to account for 3N piece

✪ Current implementation targets $J^\pi = 0^+$ states

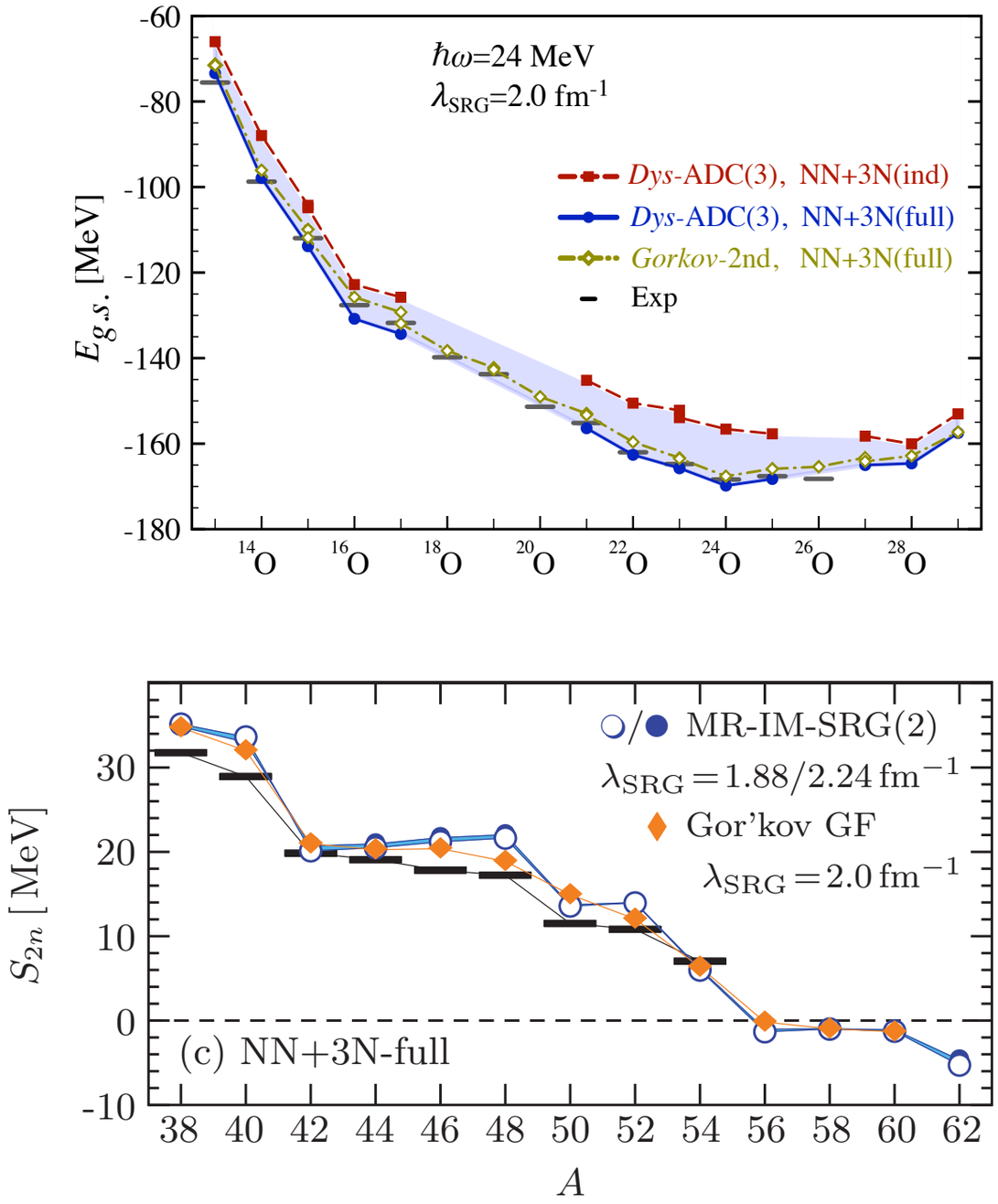
➟ Equations simplify: j-coupled scheme, block-diagonal structure, ...

➟ Odd-even g.s. energies can be accessed (through *separation energies* of A±1 systems or *perturbative blocking*)

Benchmarks

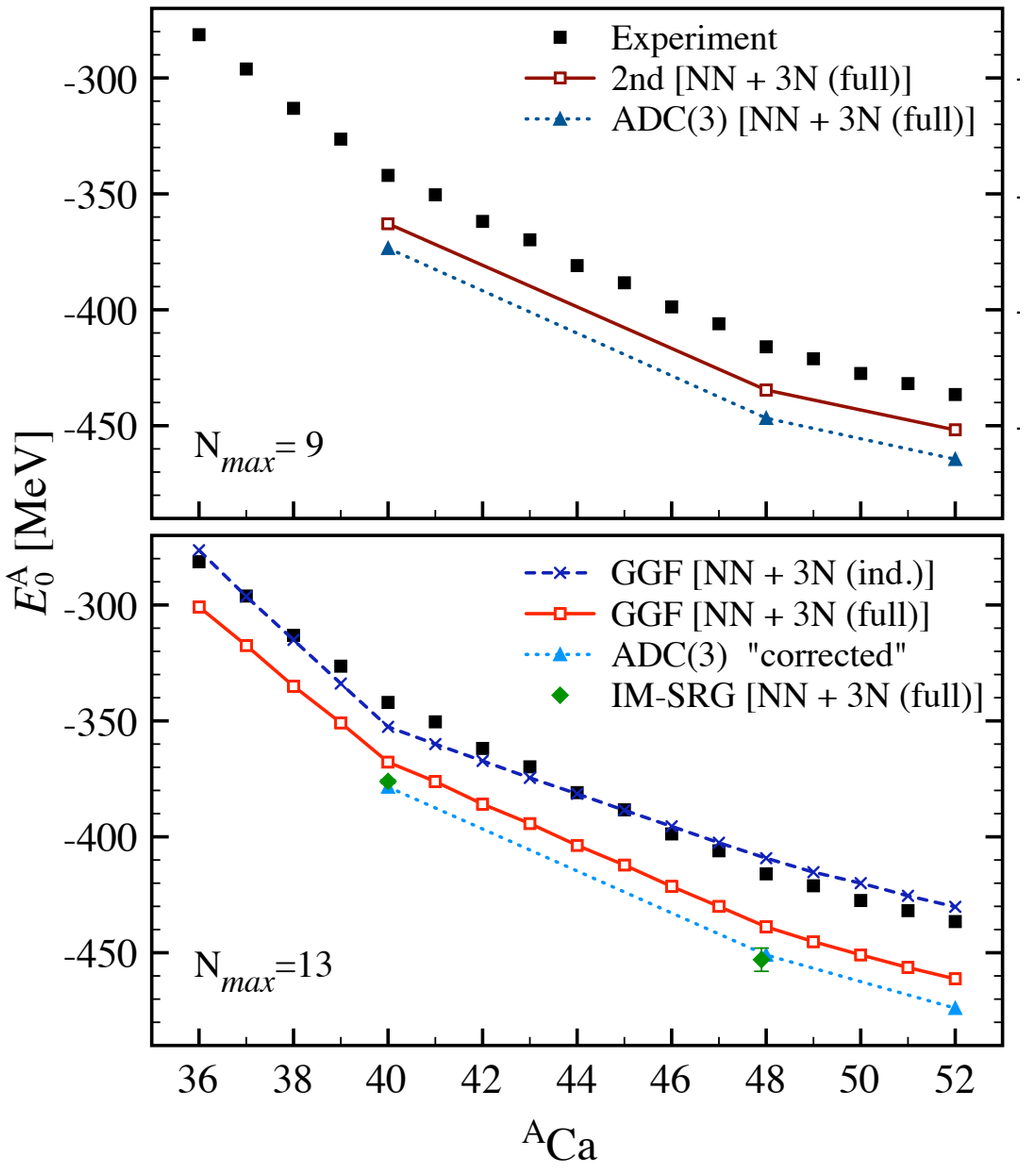
✪ Benchmarks between Gorkov GF, Dyson GF & IM-SRG

➠ Solidity of many-body machinery



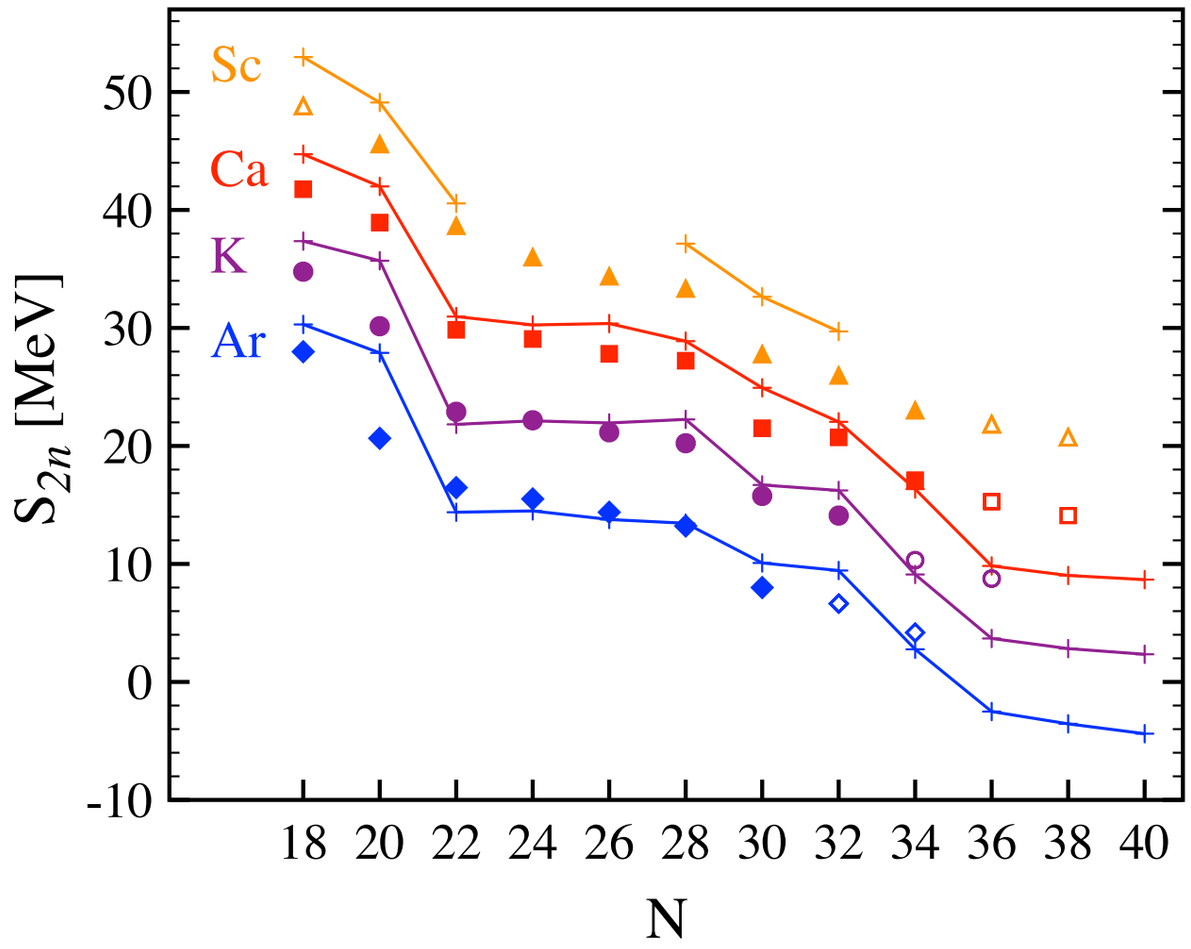
[Cipollone, Barbieri, Navrátil 2014]

[Hergert *et al.* 2014]



[Somà *et al.* 2014]

Around Ca



[Somà *et al.*, *update on* PRC 89 061301]

✪ Ab initio calculations extended to several neighbouring chains

✪ Several new experiments target neutron-rich isotopes in this mass region

✪ Calculations reveal deficiencies of employed chiral interactions

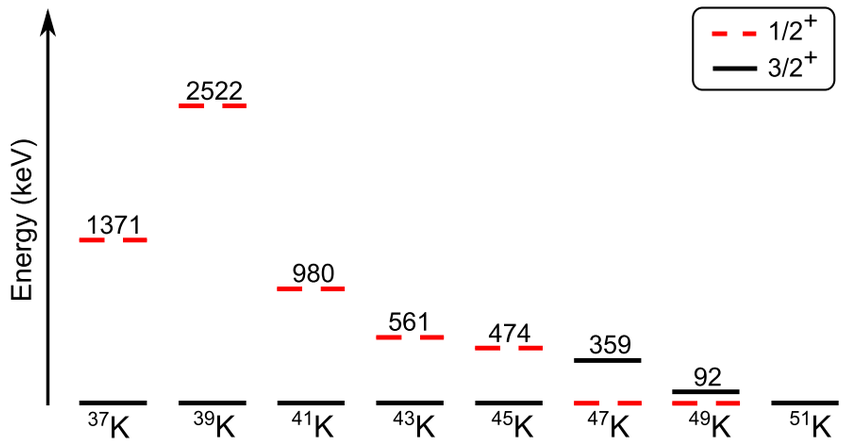
➟ Systematic overbinding & too small radii

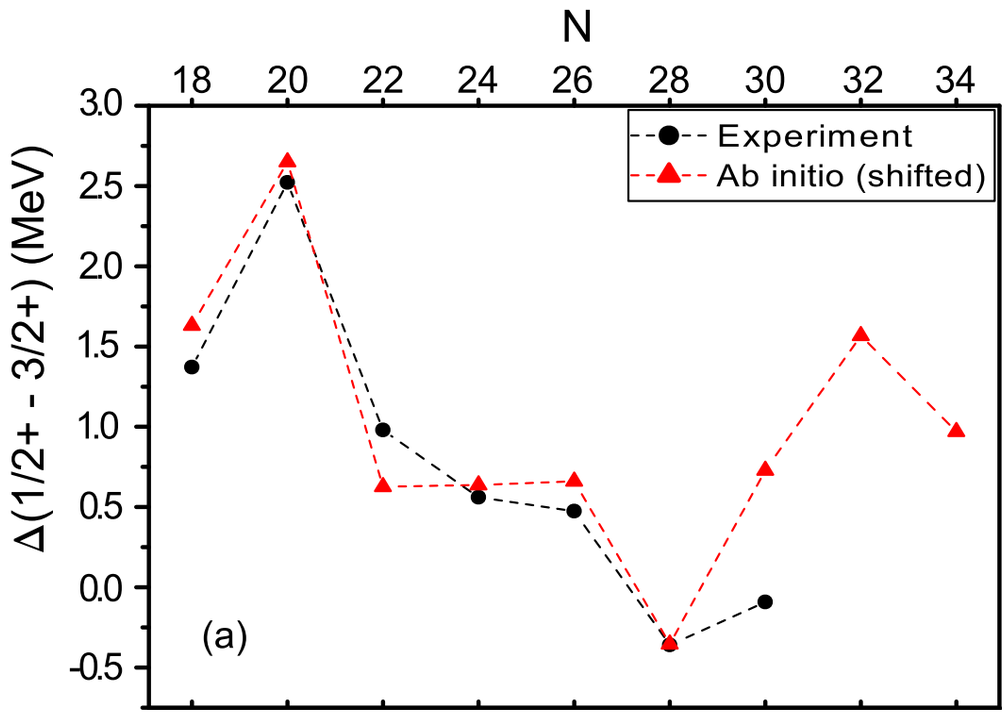
➟ Overestimation of N=20 gap traced back to spectrum too spread out

Potassium ground states (re)inversion

✪ Ground-state spin inversion & re-inversion recently established

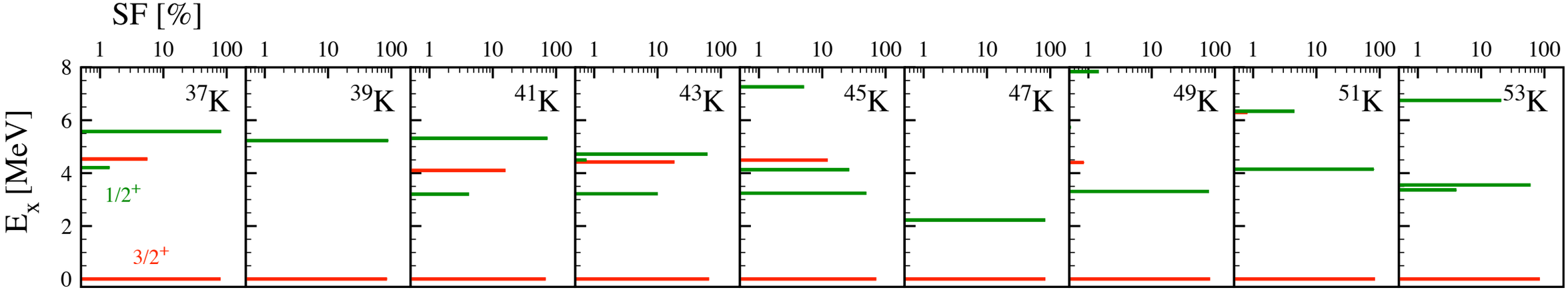
➟ Laser spectroscopy @ ISOLDE





[Papuga *et al.* 2014]

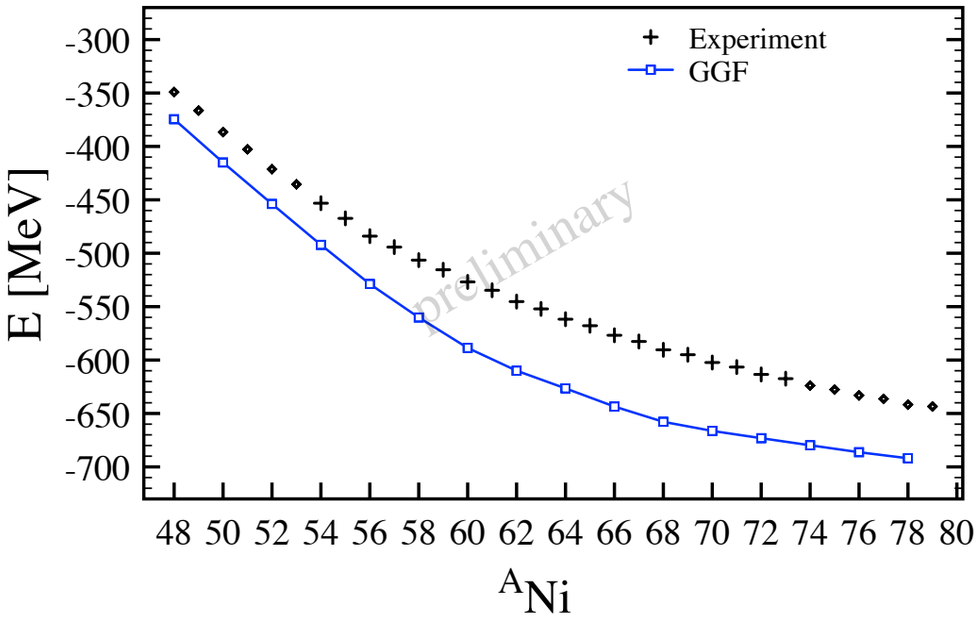
➟ GGF calculations of K spectra

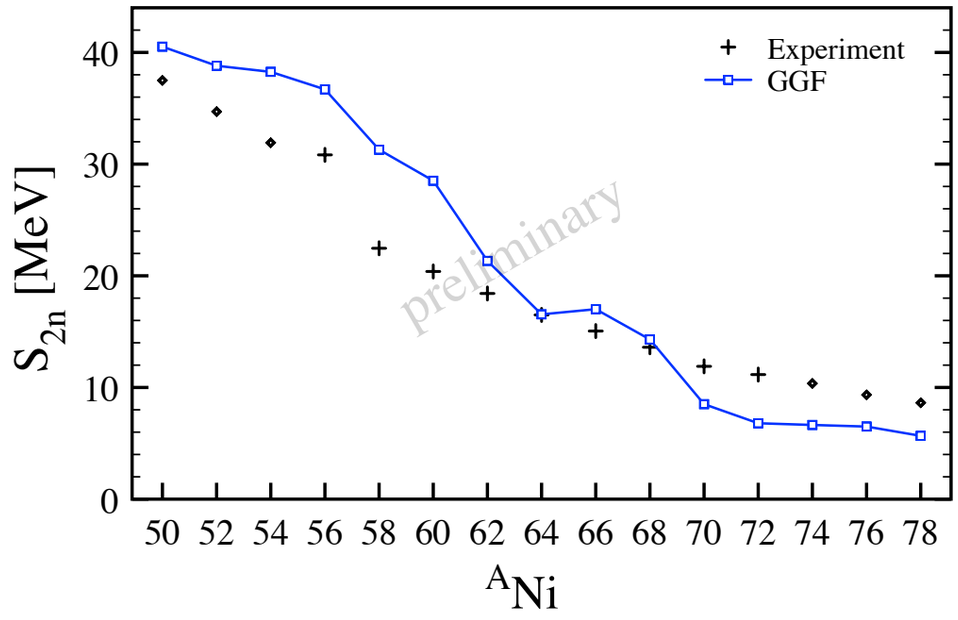


Towards heavier systems

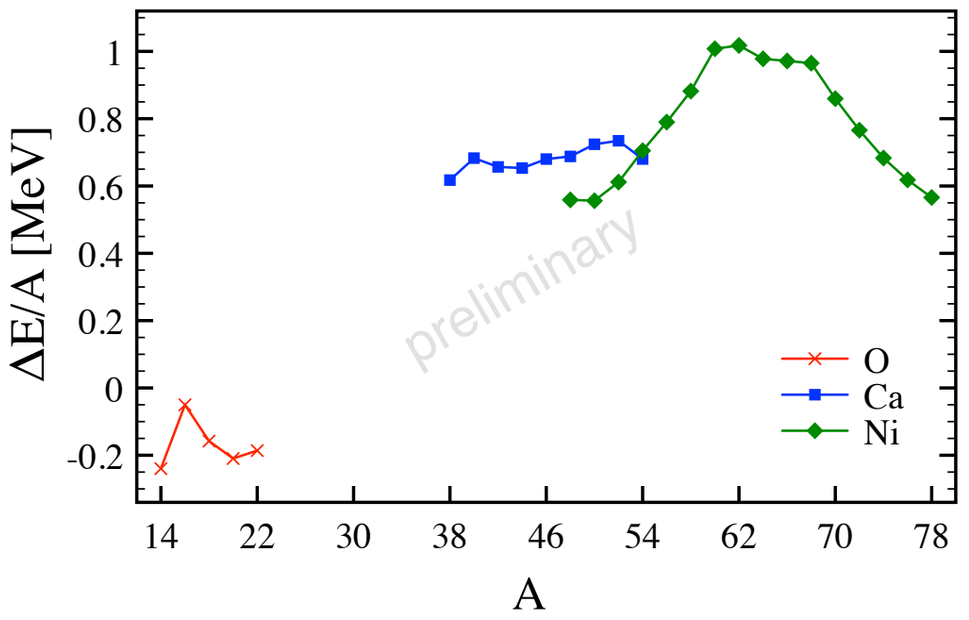
✪ Ab initio calculations being pushed towards A=100 and above

➟ Overbinding & overestimation of major shell gaps confirmed in Ni chain





[Somà *et al.*, in preparation]



➟ Confirmed by different ab initio methods

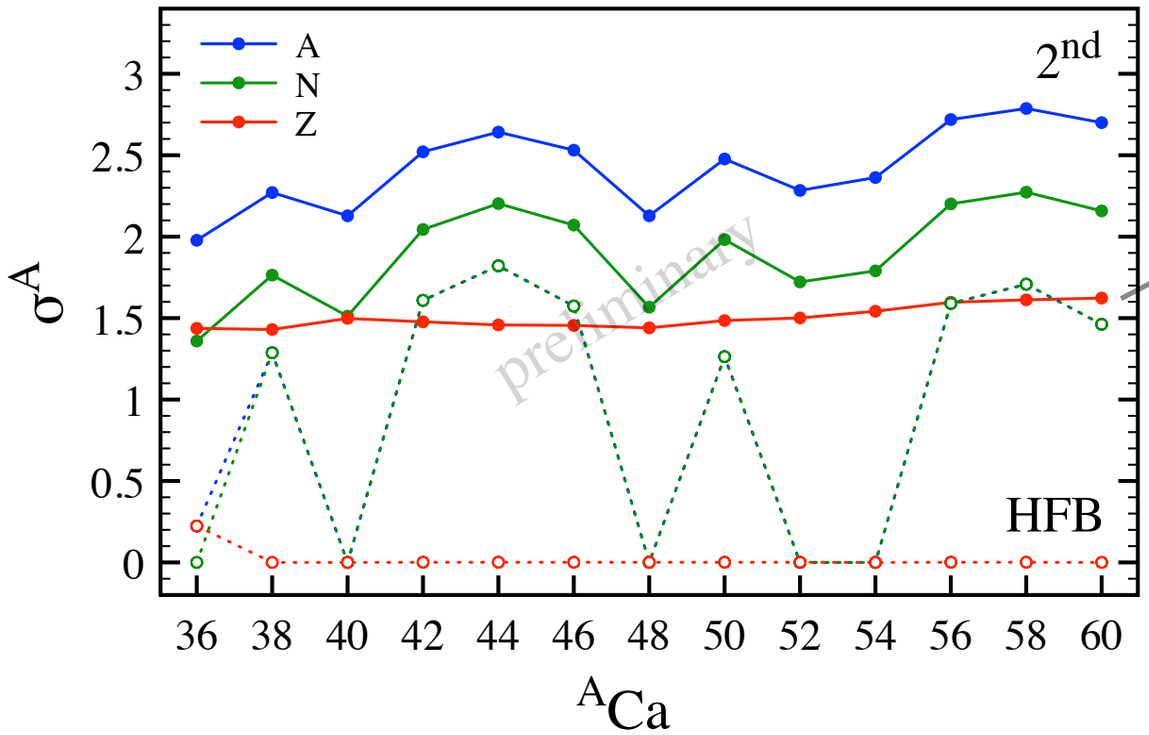
[Binder *et al.* 2014, Hergert *et al.* 2014]

Particle-number variance

- Gorkov GF calculations break particle number symmetry ⟶ $\sigma_A = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$
- Breaking has two sources:

  1) Reference state mixes different A

  2) Green's function formalism itself explores Fock space



GF breaking evident in protons

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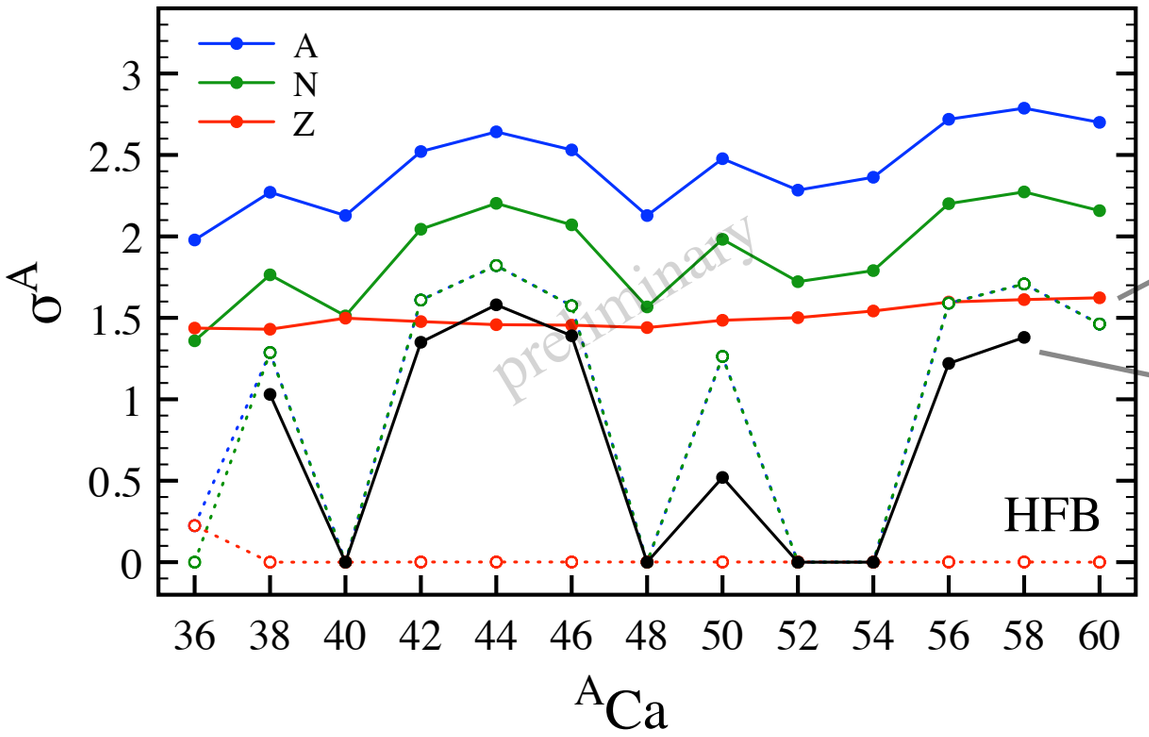

GF breaking evident in protons

After subtracting GF part

Particle-number variance

- Gorkov GF calculations break particle number symmetry ⟶ $\sigma_A = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$
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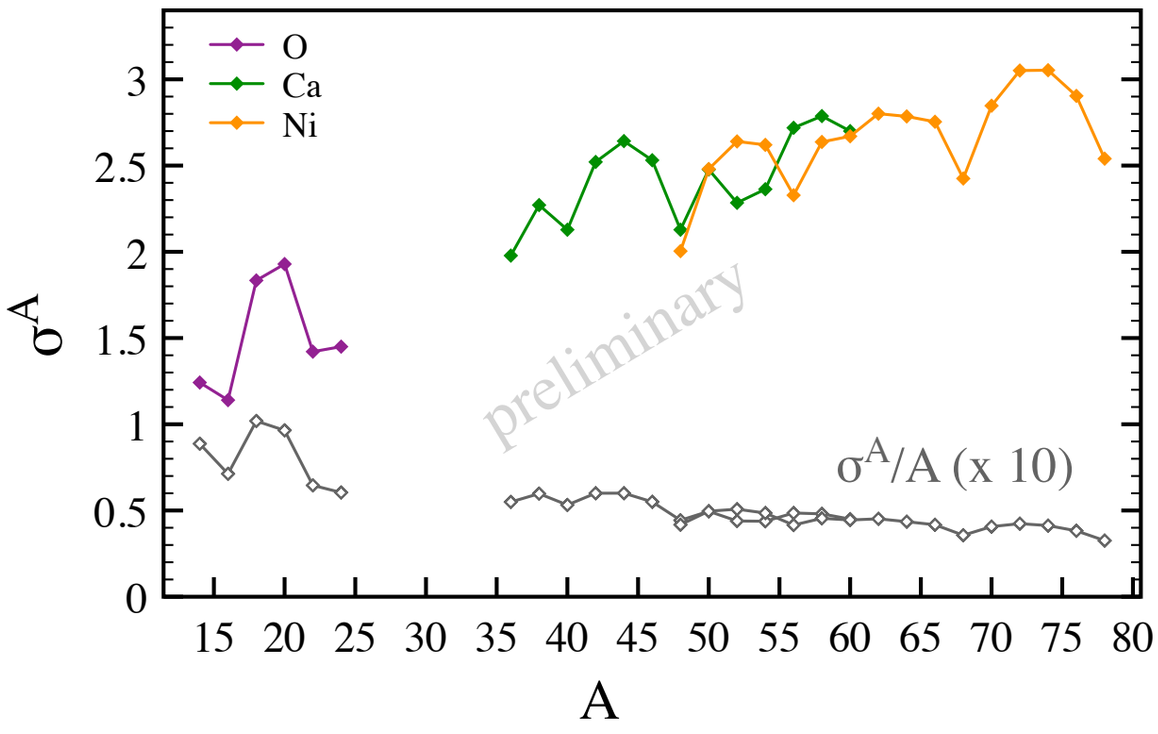

Particle-number variance

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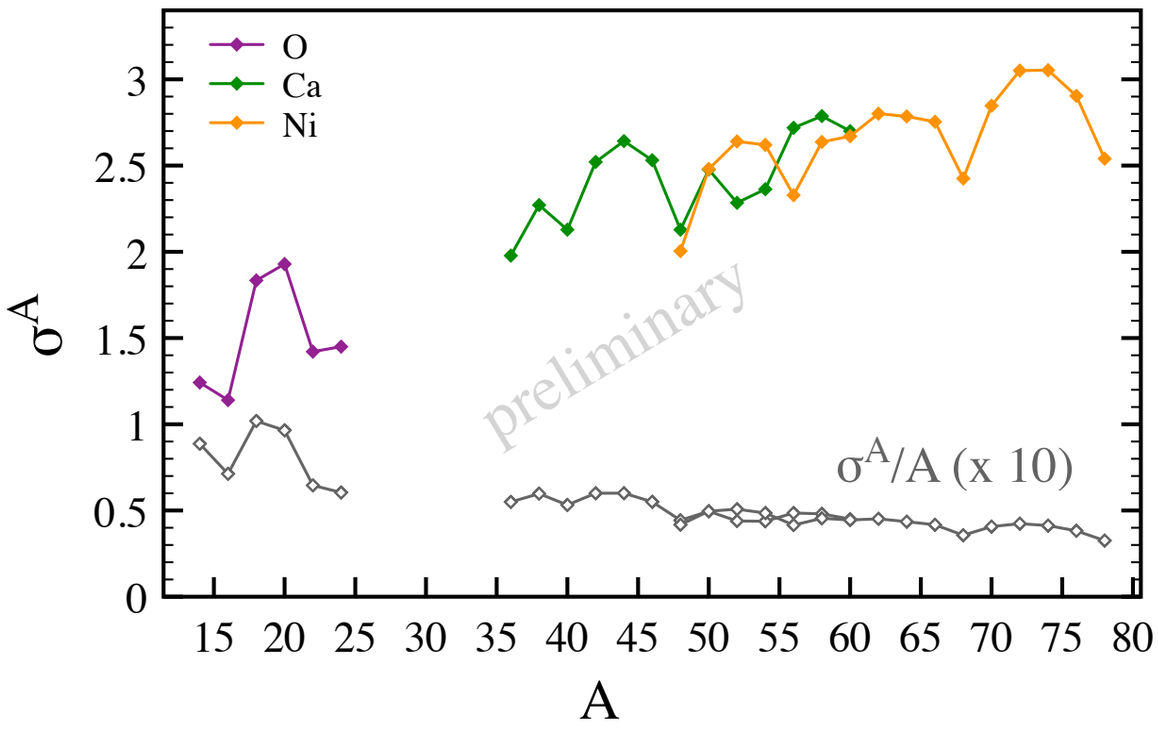


➟ Need to go beyond approximation $\rho^{(2)} \sim \rho^{(1)}\rho^{(1)}$

➟ To be further investigated at next order in GF expansion

➟ Calls for restoration of symmetry

Single-nucleon shell structure

[Duguet, Hergert, Holt, VS, arXiv:1411.1237]

✪ Reference to a **shell structure**

➟ Pillar of our understanding

➟ Provides convenient simplified picture

➪ Connection to many-body observables?

✪ Exact framework

➟ Many-body Schrödinger eq.

$$H|\Psi_k^{\mathrm{A}}\rangle = E_k^{\mathrm{A}}|\Psi_k^{\mathrm{A}}\rangle$$

➟ One nucleon addition/removal

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

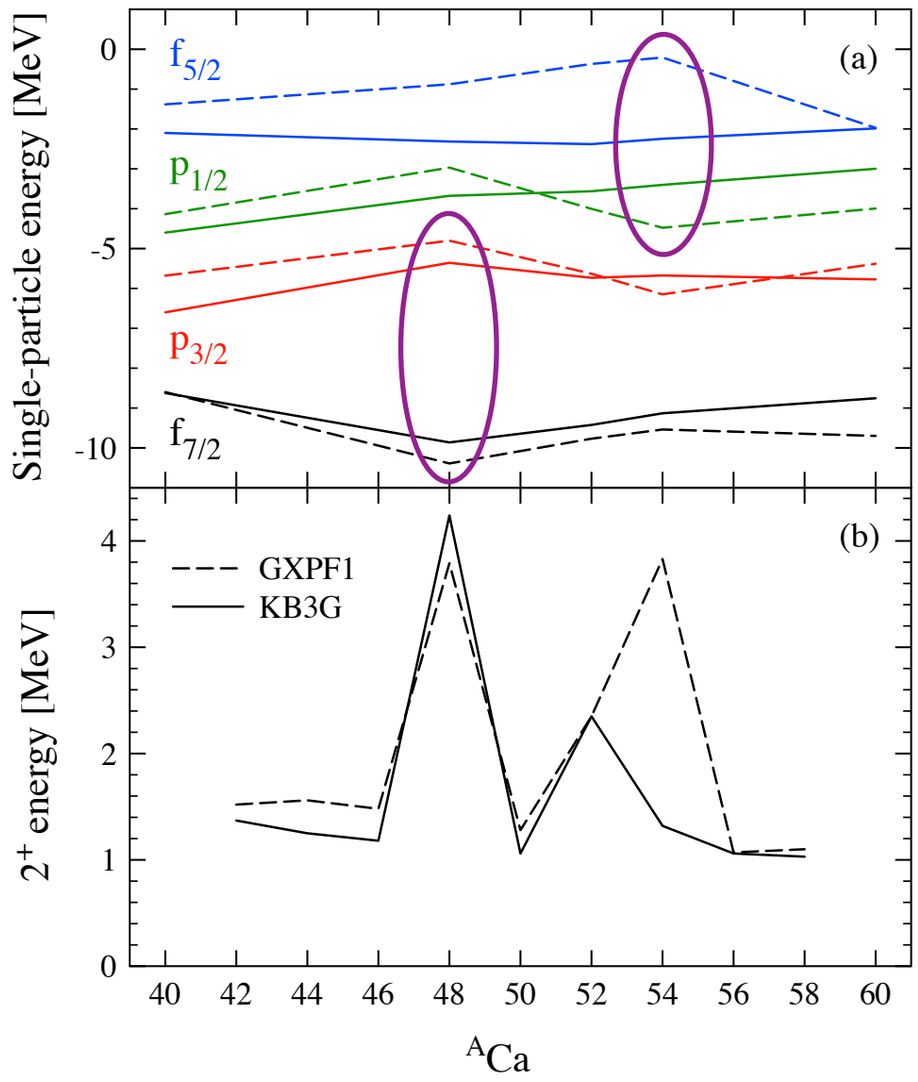
➟ Excitations, e.g. k=2_1^+

$$\Delta E^A_{0\to k} \equiv E_k^{\mathrm{A}} - E_0^{\mathrm{A}} \quad \text{and} \quad \sigma^A_{0\to k}$$

✪ Partitioning of observables

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

Empirical *pf* shell model calculations

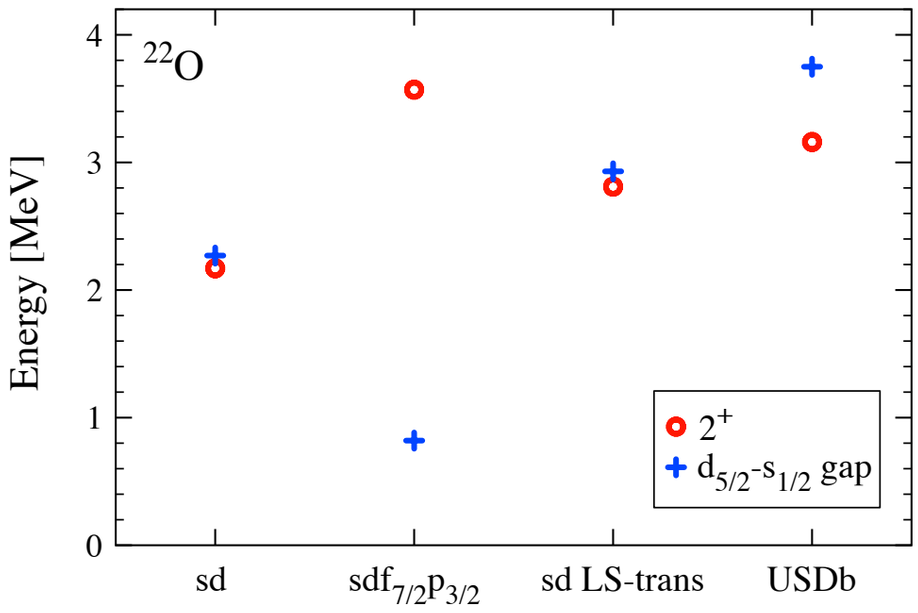


Single-nucleon shell structure

✪ Scale vs. scheme dependence

➟ **Scale**: resolution scale, unitary transformations on H

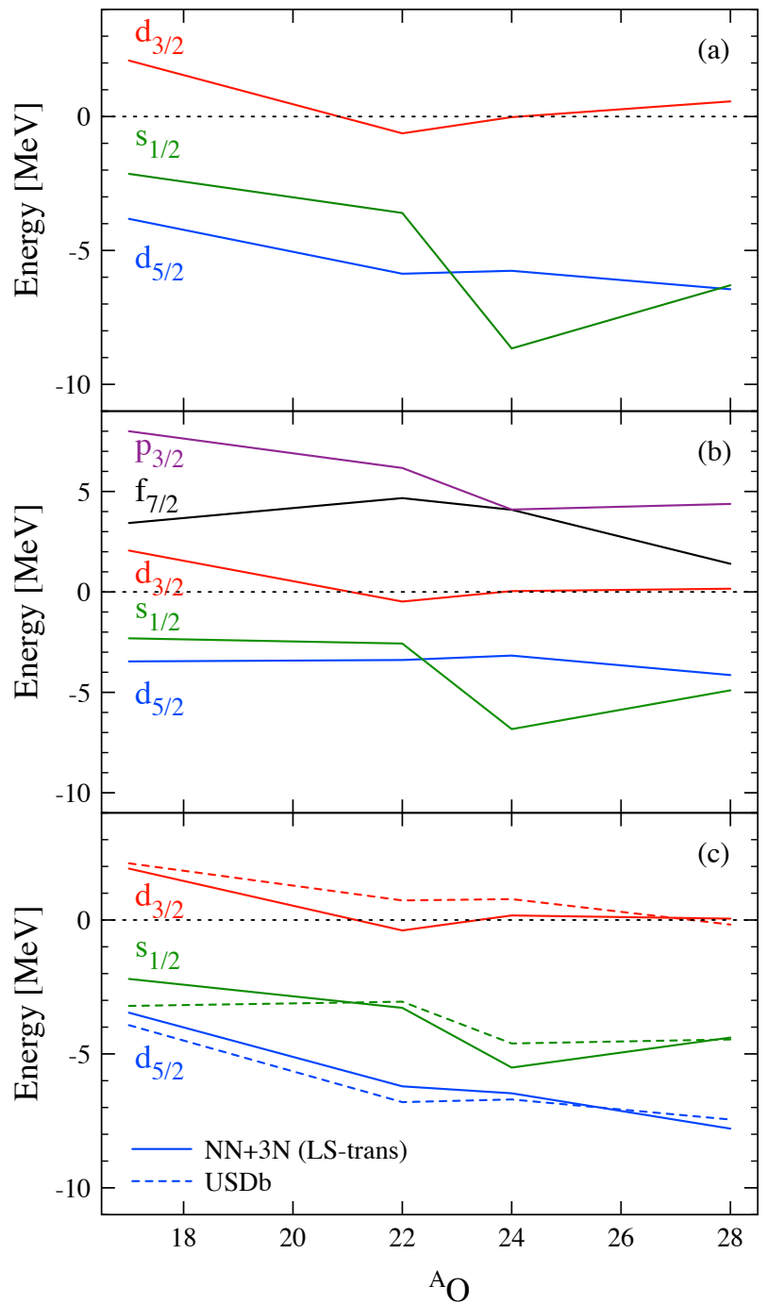
➟ **Scheme**: effective d.o.f., theoretical framework



➟ Observable essentially unchanged

➟ Correlation with s.p. gap is **scheme** dependent

Microscopic shell model calculations



Effective single-particle energies

○ Spectroscopic probability matrices

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

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

○ Spectroscopic factors

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

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

○ Sum rule & one-body centroid field

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

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

○ Effective single-particle energies

$$\mathbf{h}^{\mathrm{cent}}\, \psi_p^{\mathrm{cent}} = e_p^{\mathrm{cent}}\, \psi_p^{\mathrm{cent}}$$

$$e_p^{\mathrm{cent}} \equiv \sum_{\mu \in \mathcal{H}_{A+1}} S_\mu^{+pp} E_\mu^+ + \sum_{\nu \in \mathcal{H}_{A-1}} S_\nu^{-pp} E_\nu^-$$

[Baranger 1970]

➟ Defined solely from output of the Schrödinger eq.

➟ Computable in any many-body scheme

➟ Physically relates to the averaged dynamics of nucleons

➟ Reduces to HF s.p. energies in HF approximation

Effective single-particle energies

○ Spectroscopic probability matrices

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

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under a unitary transformation U(λ)

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

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

Ab initio setup & breaking of unitarity

- Calculations in oxygen isotopes
- Two different ab initio methods (Gorkov GF & MR-IM-SRG)
- NN & 3N chiral interactions SRG-evolved to 1.88, 2.0, 2.24 fm^{-1}

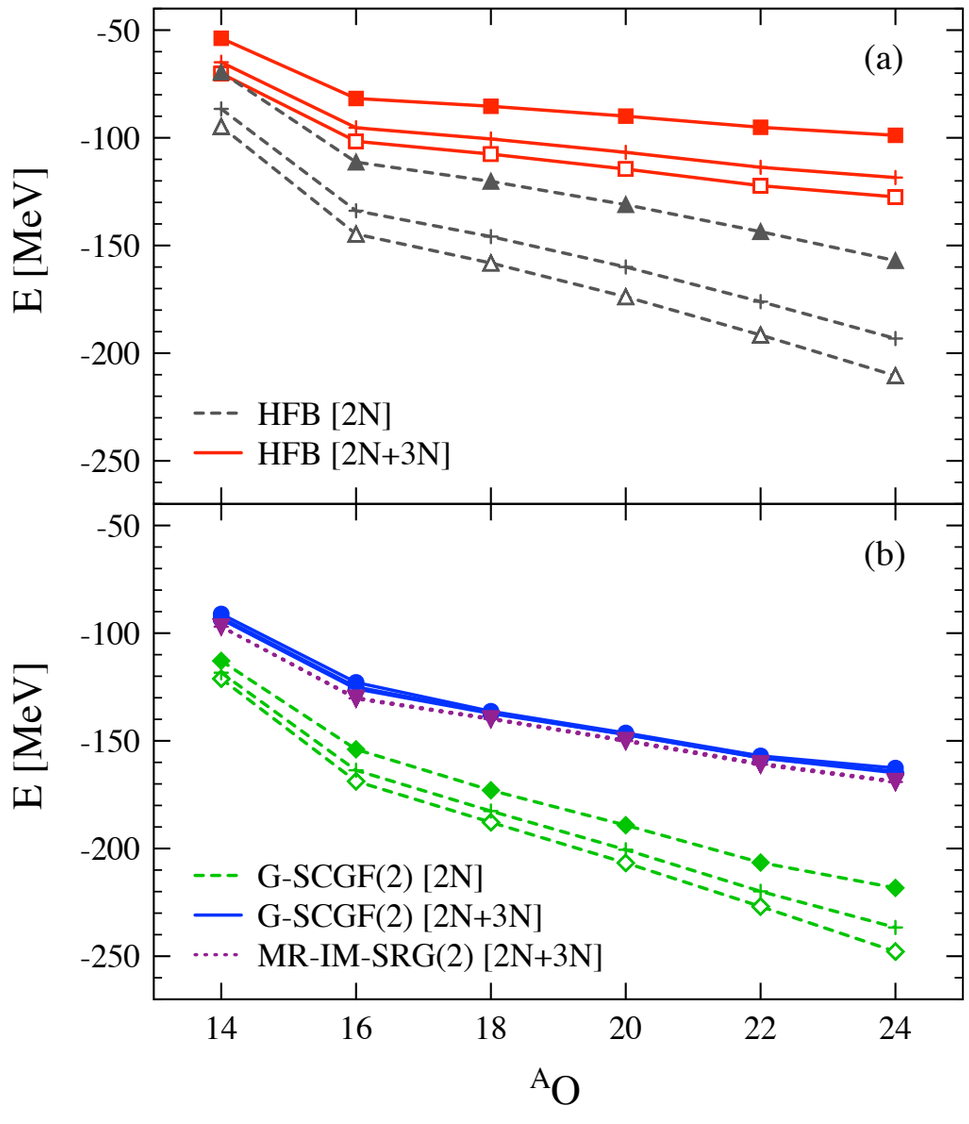
✪ Breaking of unitarity: origin

➟ Omit $V^{AN}(\lambda)$ for A>3

➟ Approximate the solution of Schr. eq.

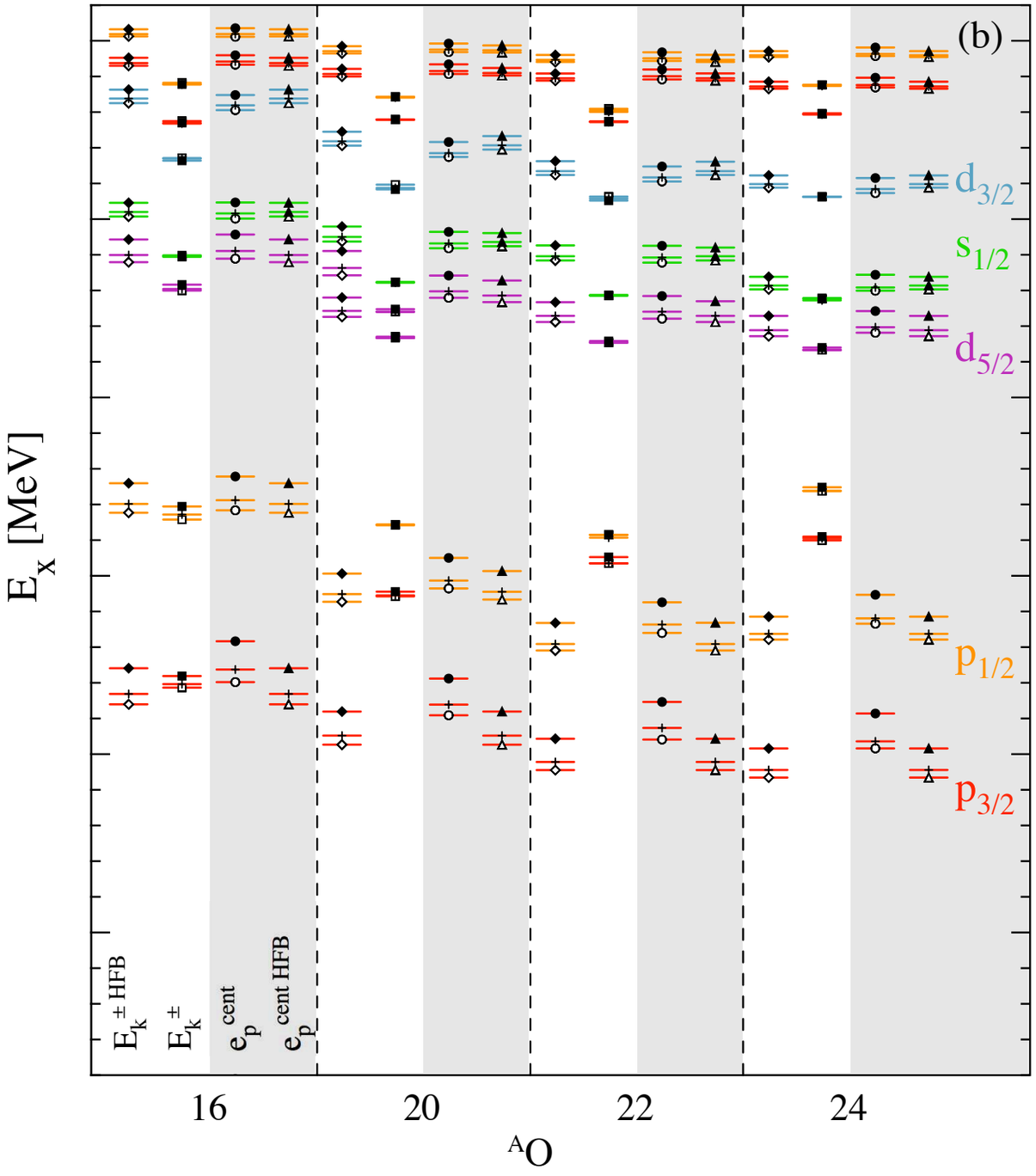
✪ Consequence

➟ Artificial running of observables

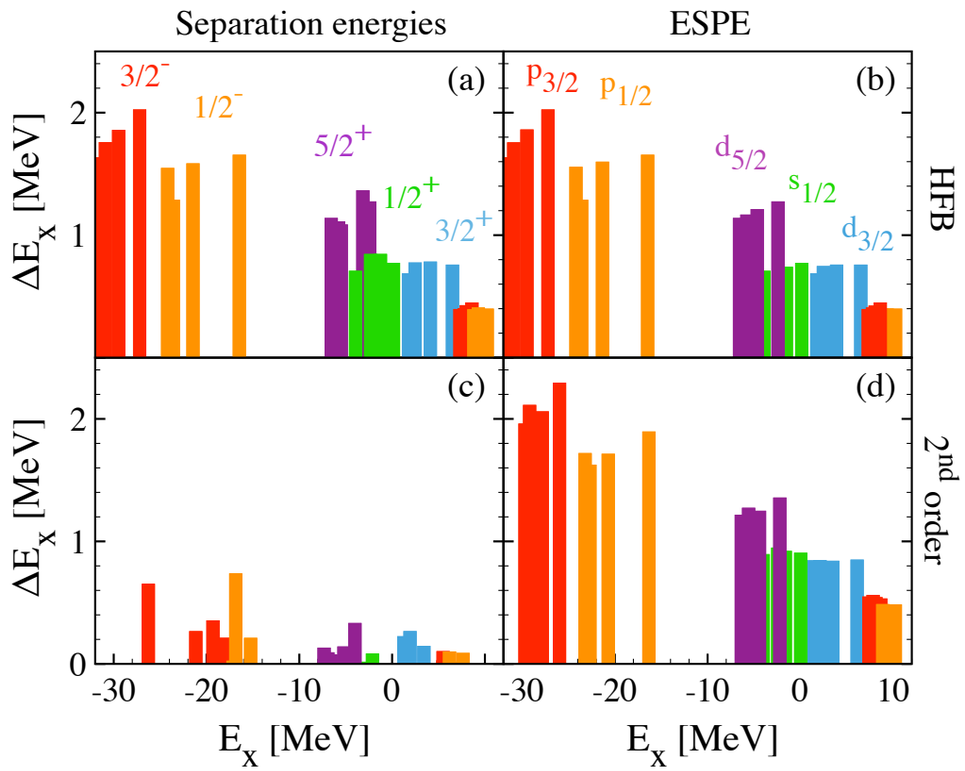


Non-observability of shell structure

✪ One-nucleon separation energies vs. ESPEs



Residuals



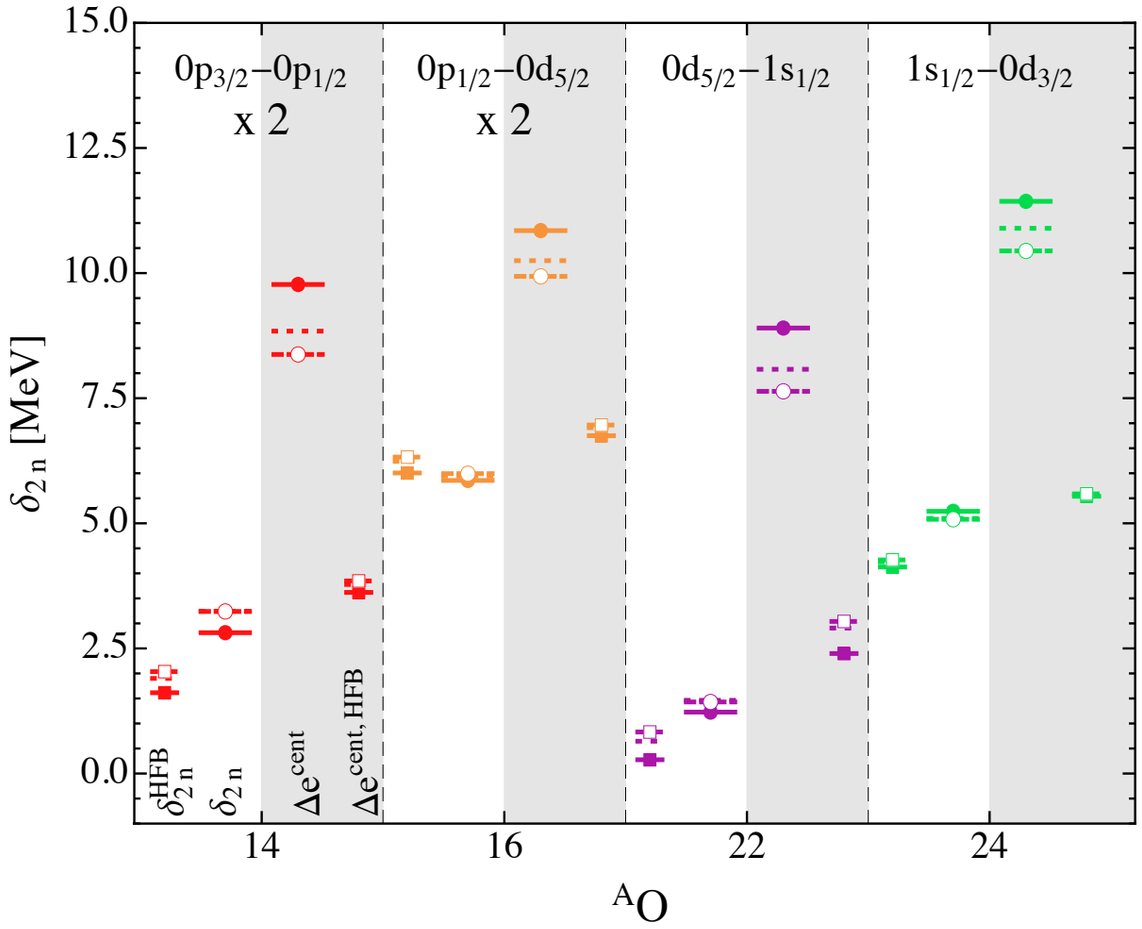
➟ Spread of sep. en. reduced significantly

➟ Spread of ESPEs unchanged

Non-observability of shell structure

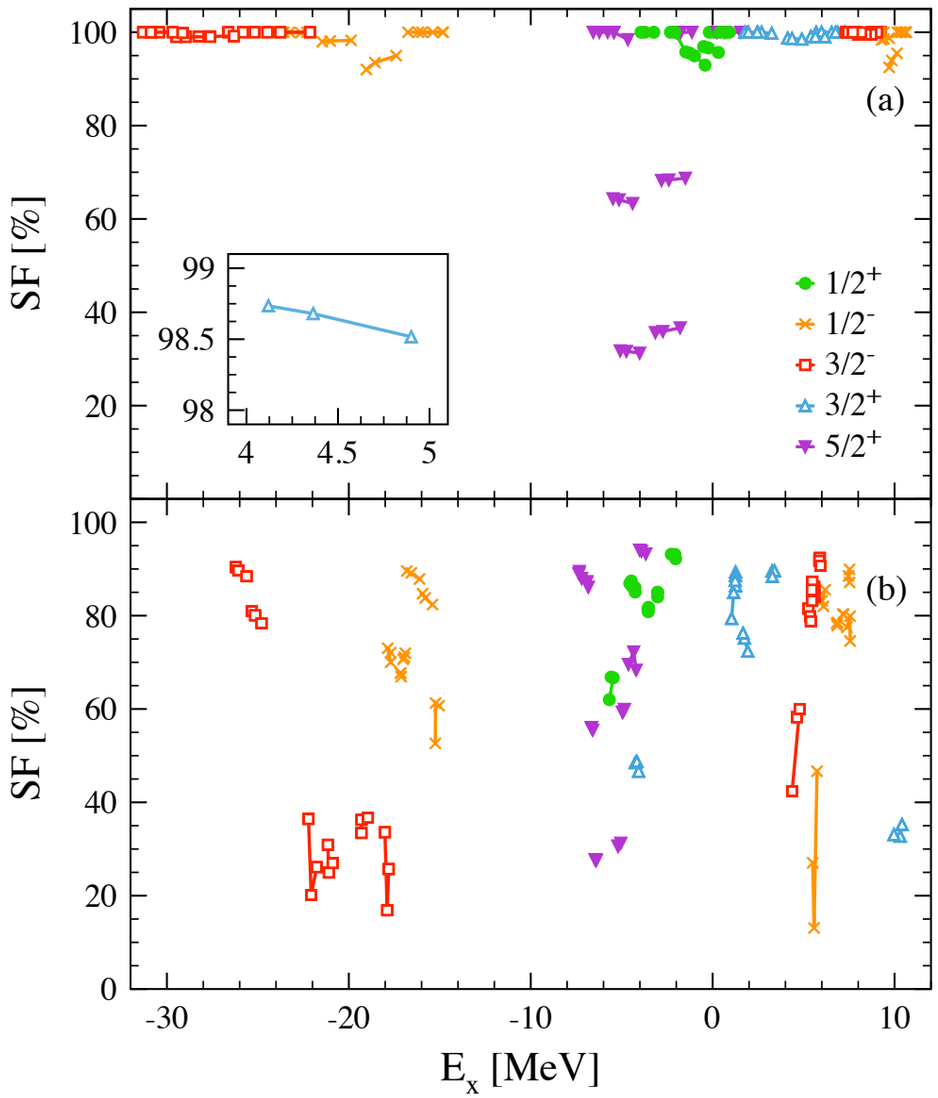
Two-neutron shell gap $\delta_{2n}(N,Z) \equiv \frac{1}{2}\left[E(N+2,Z) - 2E(N,Z) + E(N-2,Z)\right]$

vs. ESPE Fermi gap $\Delta e_{\mathrm{F}}^{\mathrm{cent}}(N,Z) \equiv e_p^{\mathrm{cent}}(N,Z) - e_h^{\mathrm{cent}}(N,Z)$



Limited running with $\lambda \in [1.88, 2.36]$ fm^{-1}

Spectroscopic factors



Summary

✪ Ab initio calculations able to address **several mid-mass isotopic chains**

➟ Provide a stringent test ground for nuclear interactions

✪ Relative quantities already well described along a chain

✪ Particle number variance calls for **symmetry restored theory**

✪ Non-observability of shell structure

➟ Correlations between observables & shell structure **depend on the resolution scale**

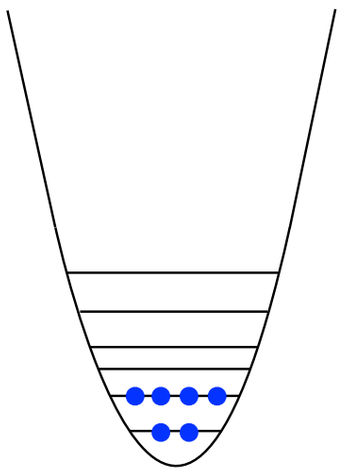
➟ Scale/scheme dependence should be explicit & consistent

➟ **Quantification of scale dependence** interesting from a pragmatic point of view

Appendix

Different ab initio strategies

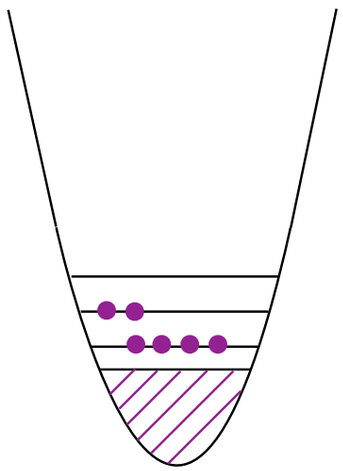
Light nuclei



Virtually exact

NCSM, GFMC, ...

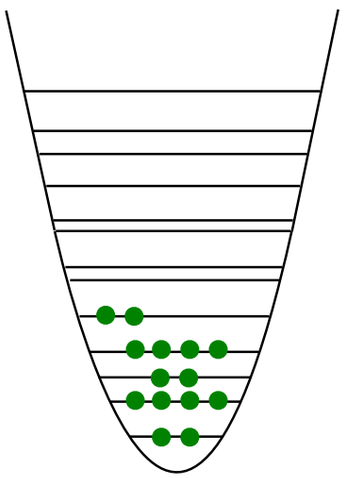
Medium-mass nuclei



Valence space

Microscopic SM

Mid/heavy nuclei



Based on expansion

GF, CC, IM-SRG, ...

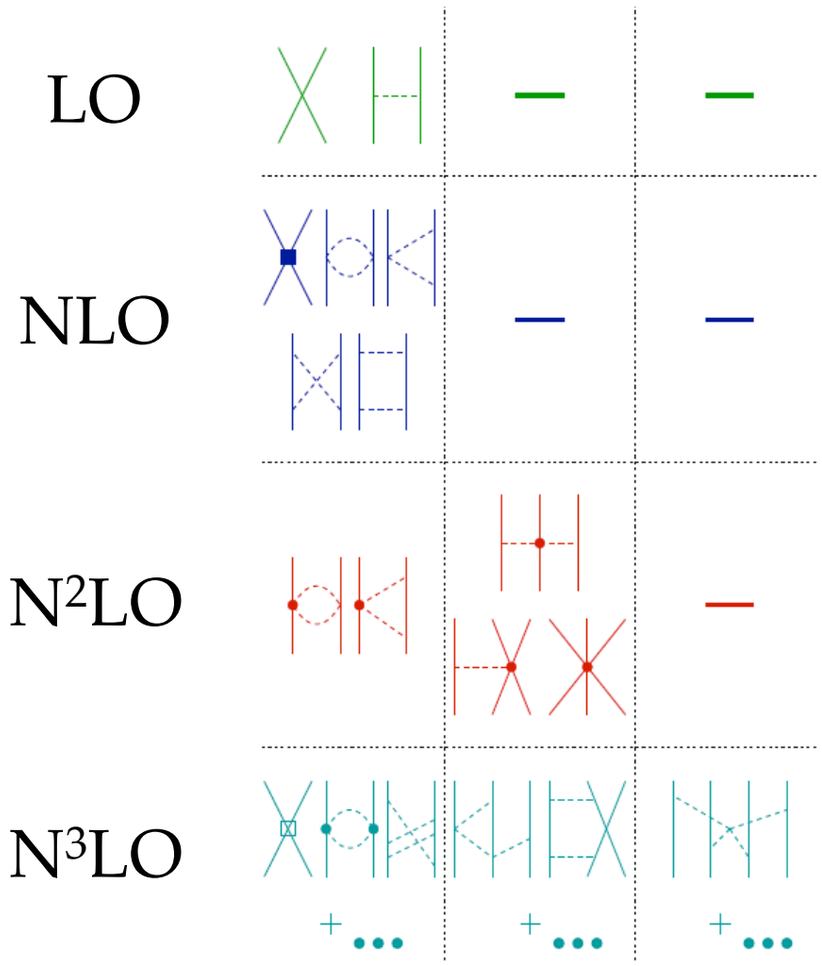
Closed-shell

Open-shell

All methods (should be able to) take the same input Hamiltonian

➟ Alternative approach: lattice EFT

Chiral EFT & inter-nucleon interactions



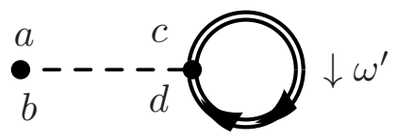
- ✪ Separation of scales
- ✪ Expansion in powers of momenta
- ✪ Long-range physics explicit
  +
  Short-range couplings
- ✪ Consistent many-body forces
- ✪ Systematic, provides error estimates

- ✪ Very promising, but yet not completely satisfactory
  - ➟ Different orders in EFT
  - ➟ Consistency of cutoffs?
  - ➟ Order-by-order convergence unclear
  - ➟ More fundamental problem: EFT power counting

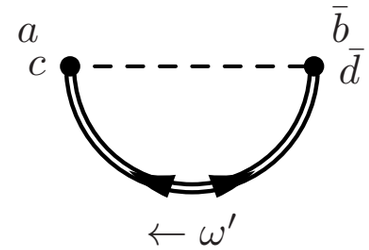
Gorkov equation & self-energy expansion

✪ 1st order ➟ energy-independent self-energy

$$\Sigma^{11\,(1)}_{ab} =$$

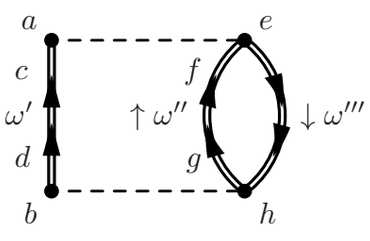


$$\Sigma^{12\,(1)}_{ab} =$$



✪ 2nd order ➟ energy-dependent self-energy

$$\Sigma^{11\,(2)}_{ab}(\omega) =$$



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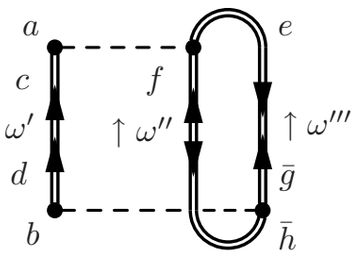
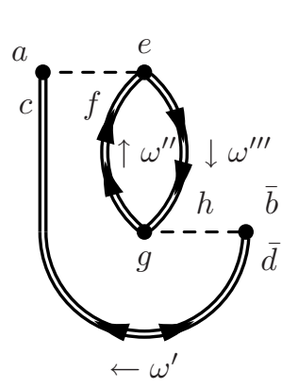


$$\Sigma^{12\,(2)}_{ab}(\omega) =$$



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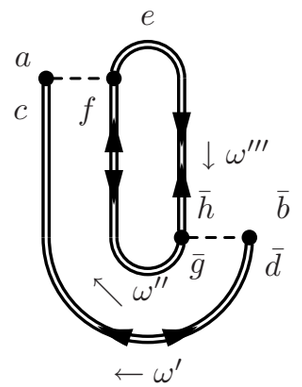
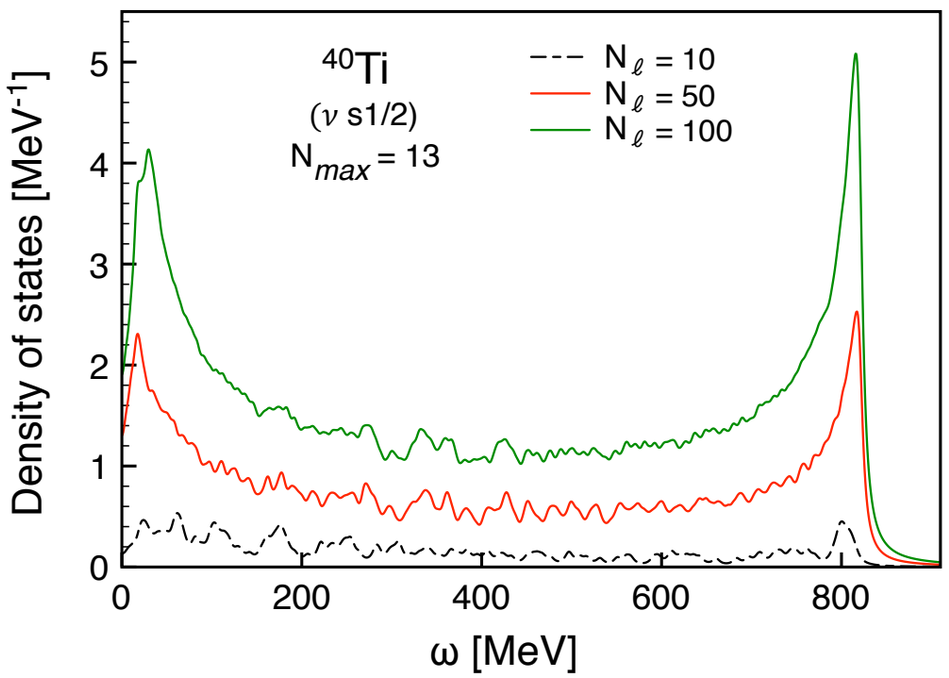


energy *independent* eigenvalue problem

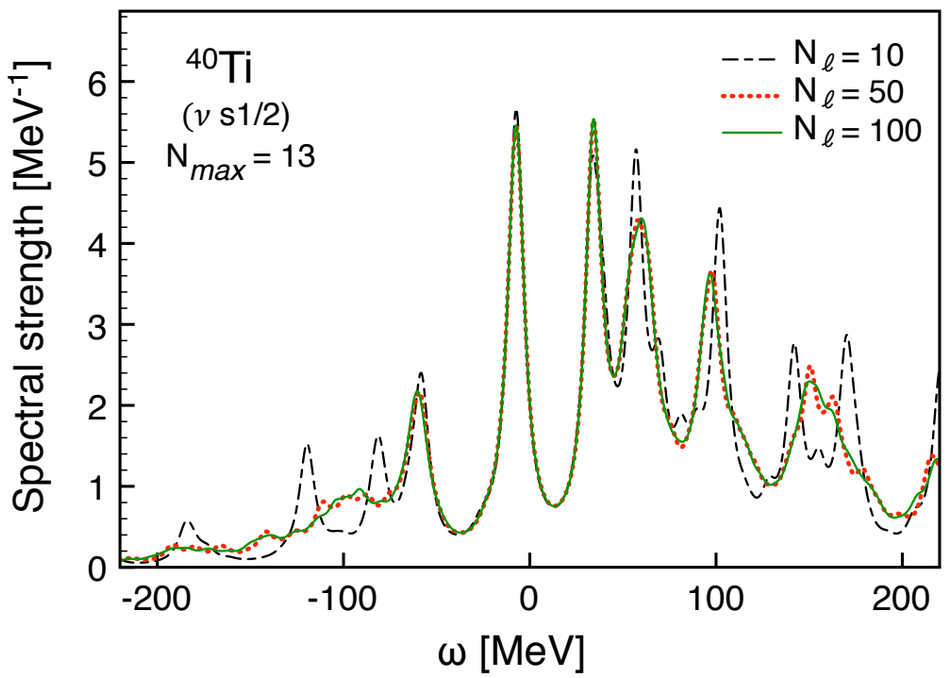
$$\begin{pmatrix} T-\mu+\Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^\dagger \\ \tilde{h}^\dagger & -T+\mu-\Lambda & -\mathcal{D}^\dagger & \mathcal{C} \\ \mathcal{C}^\dagger & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^\dagger & 0 & -E \end{pmatrix} \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix}$$

Testing Krylov projection & model space truncation

Density of states



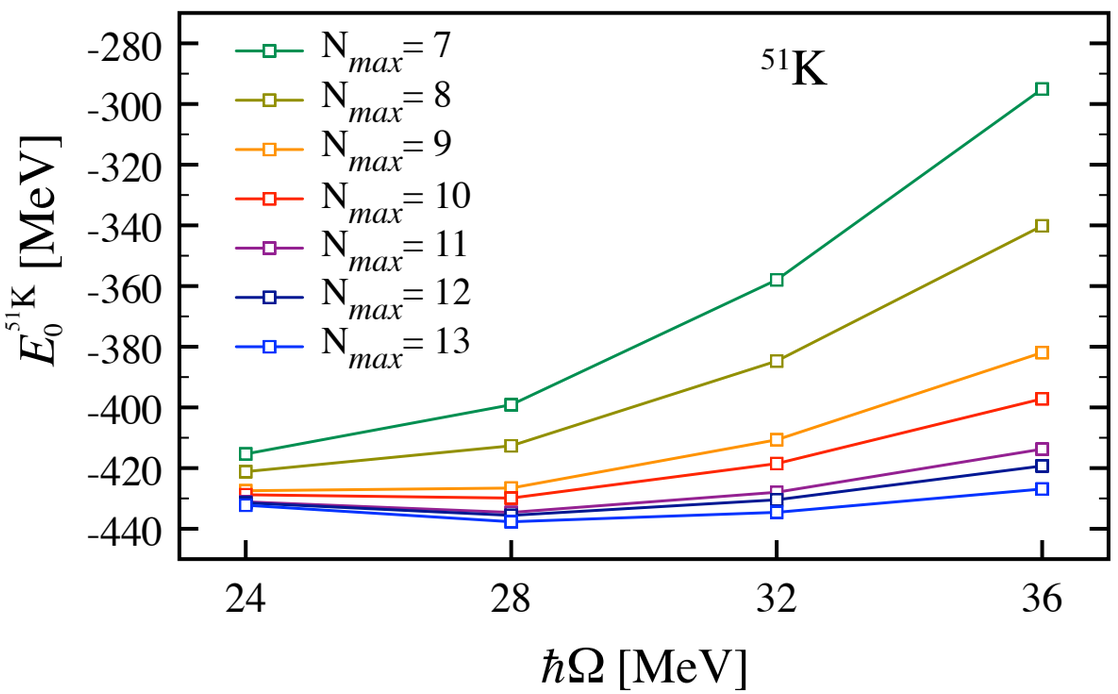
Spectral strength



[Somà, Barbieri & Duguet 2014]

Krylov projection well under control

Error from model space truncation around 1 MeV



Odd-even systems

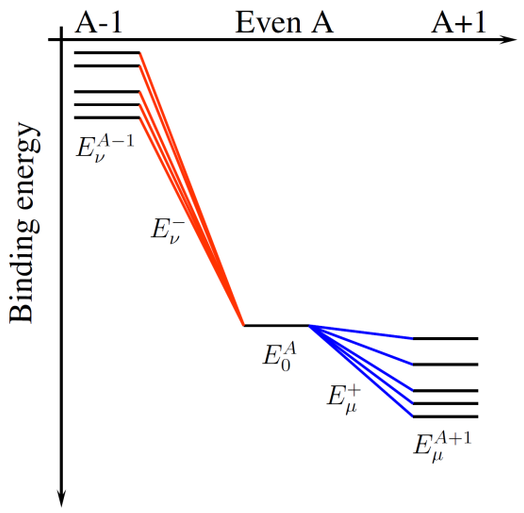
✪ Current implementation targets $J^\pi = 0^+$ states

➟ Equations simplify: j-coupled scheme, block-diagonal structure, ...

✪ Different possibilities to compute odd-even g.s. energies:

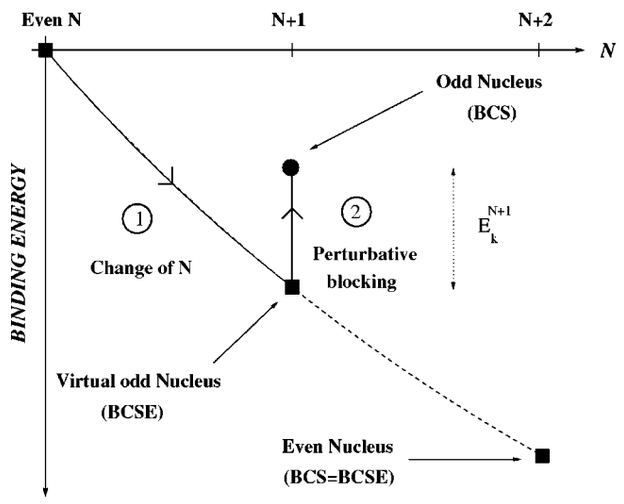
① From separation energies

➟ Either from A-1 or A+1



② From fully-paired even number-parity state

➟ "Fake" odd-A plus correction



[Duguet *et al.* 2001]

Two methods agree within 2-300 keV

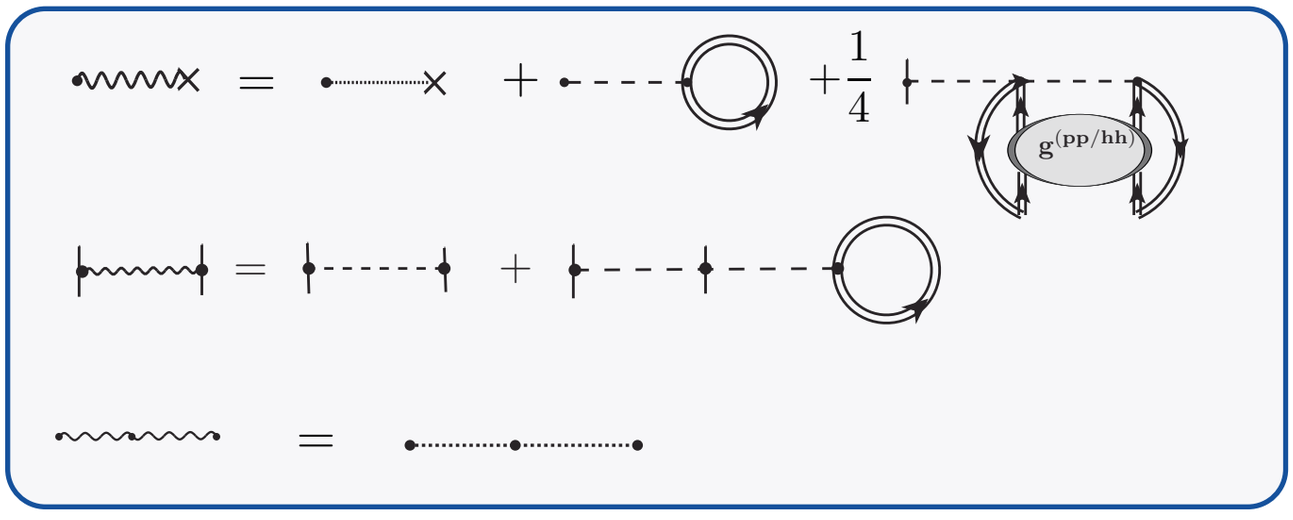
Three-body forces

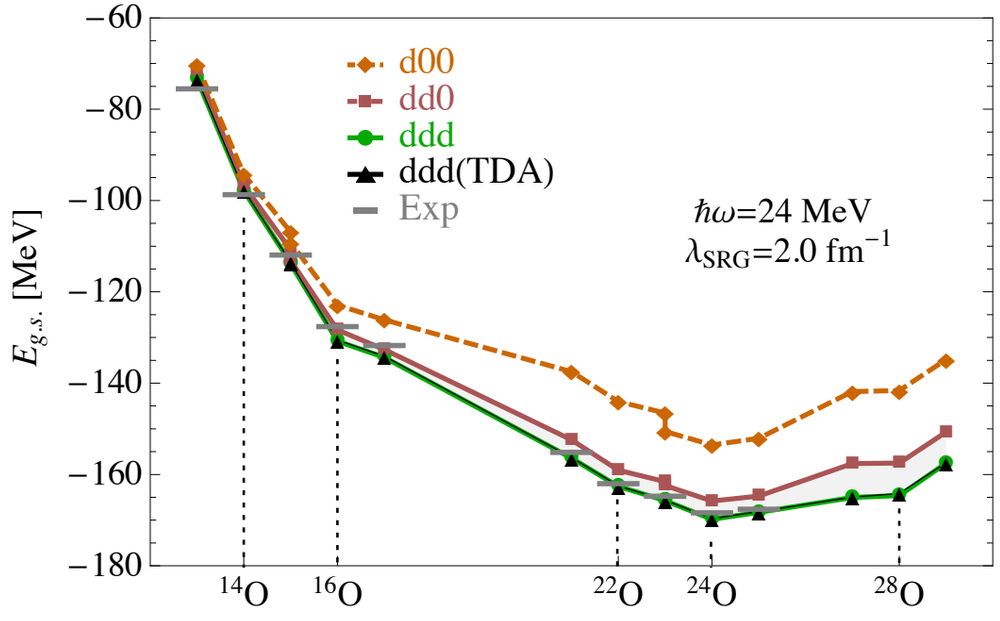
✪ One- and two-body forces derived from the 3N part of the Hamiltonian

➟ Contractions with fully correlated density matrix

➟ Generalization of normal ordering

✪ Galitskii-Koltun sum rule modified to account for 3N piece





[Cipollone *et al.* 2013]

➟ Use of dressed propagators provides extra correlations

Choice of NN+3N potential

✪ NN potential:

○ chiral N^3LO (500 MeV)

➟ SRG-evolved to 2.0 fm^{-1}

[Entem and Machleidt 2003]

✪ 3N potential:

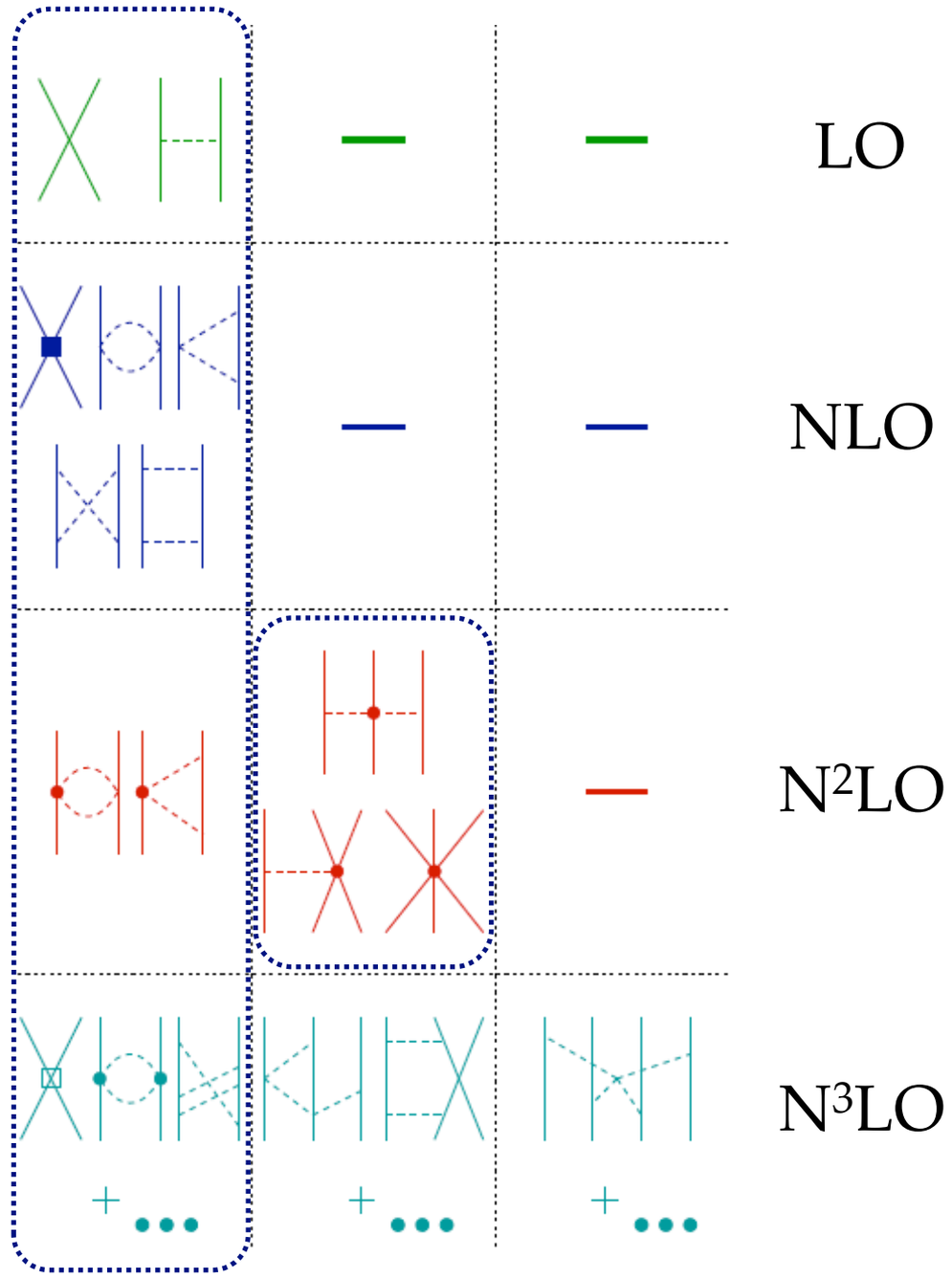
○ chiral N^2LO (400 MeV)

➟ SRG-evolved to 2.0 fm^{-1}

[Navrátil 2007]

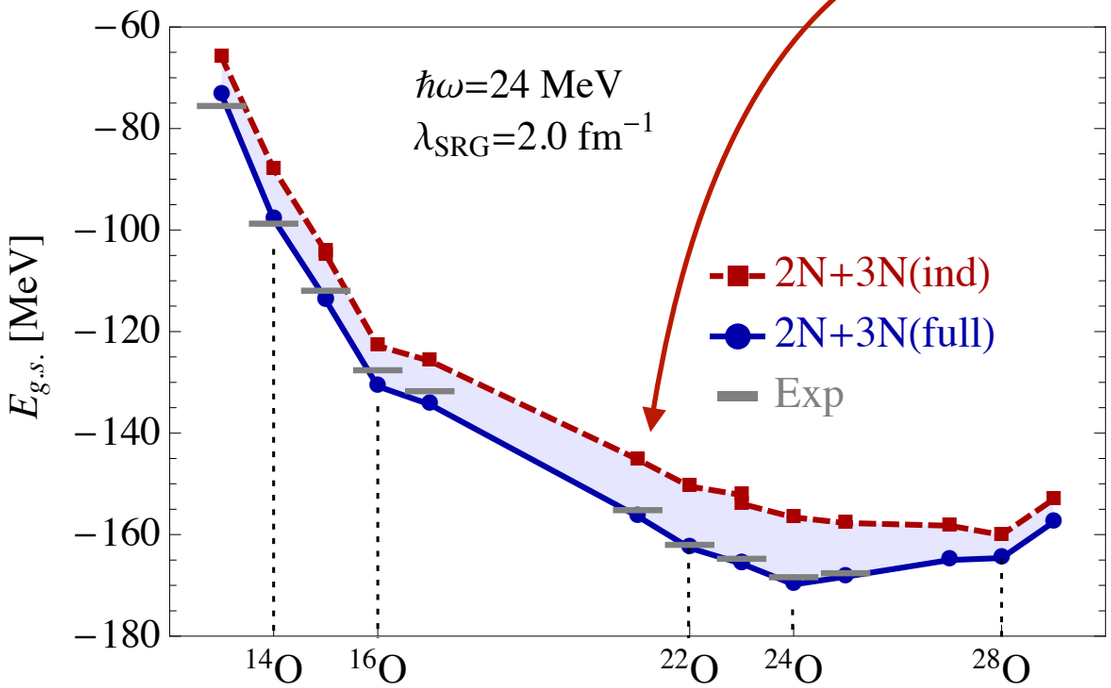
➟ Choice of cutoff to reduce induced 4N contributions

[Roth *et al*. 2012]

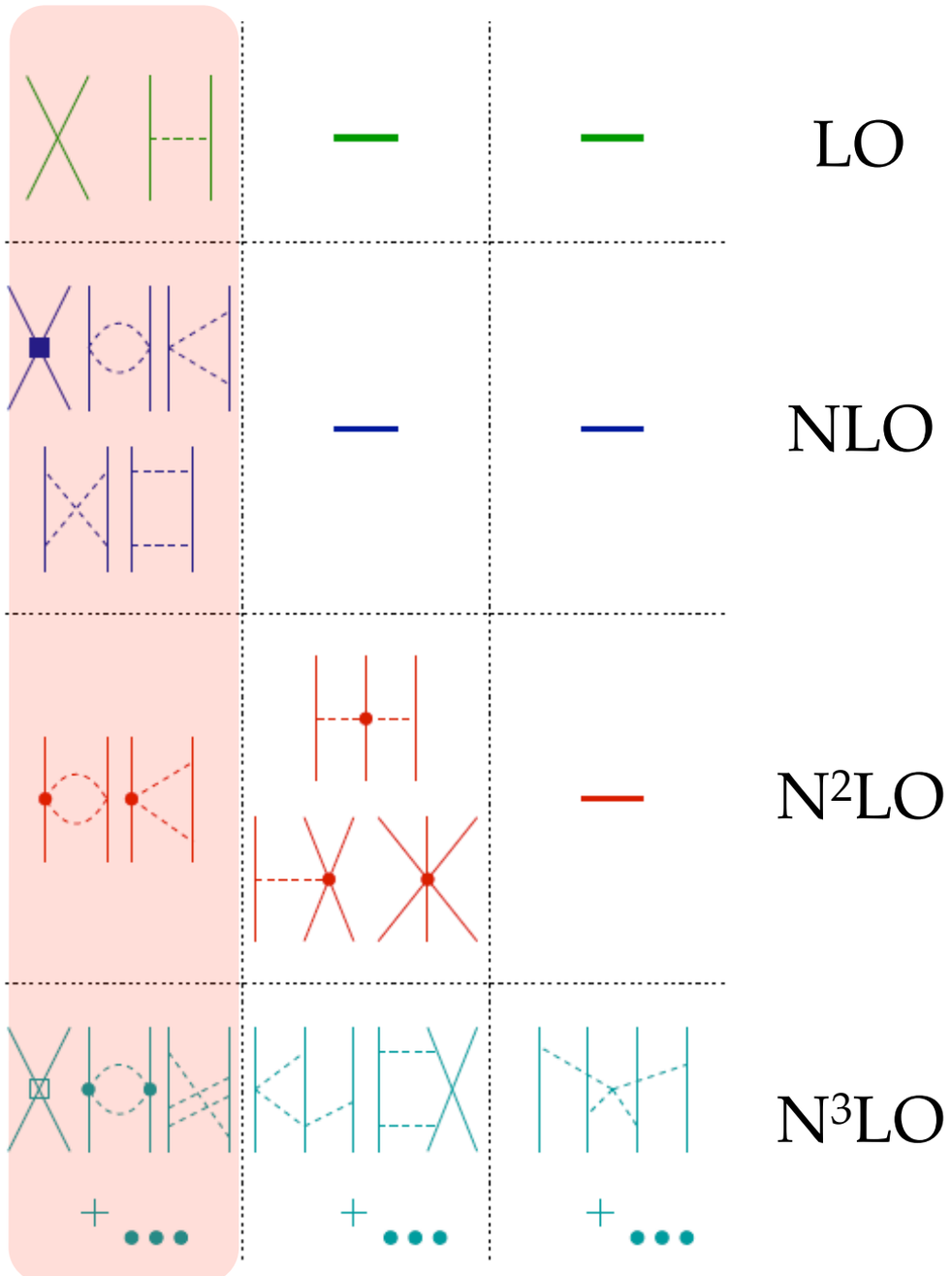


Chiral NN+3N in the oxygen chain

✪ Self-consistent Green's functions

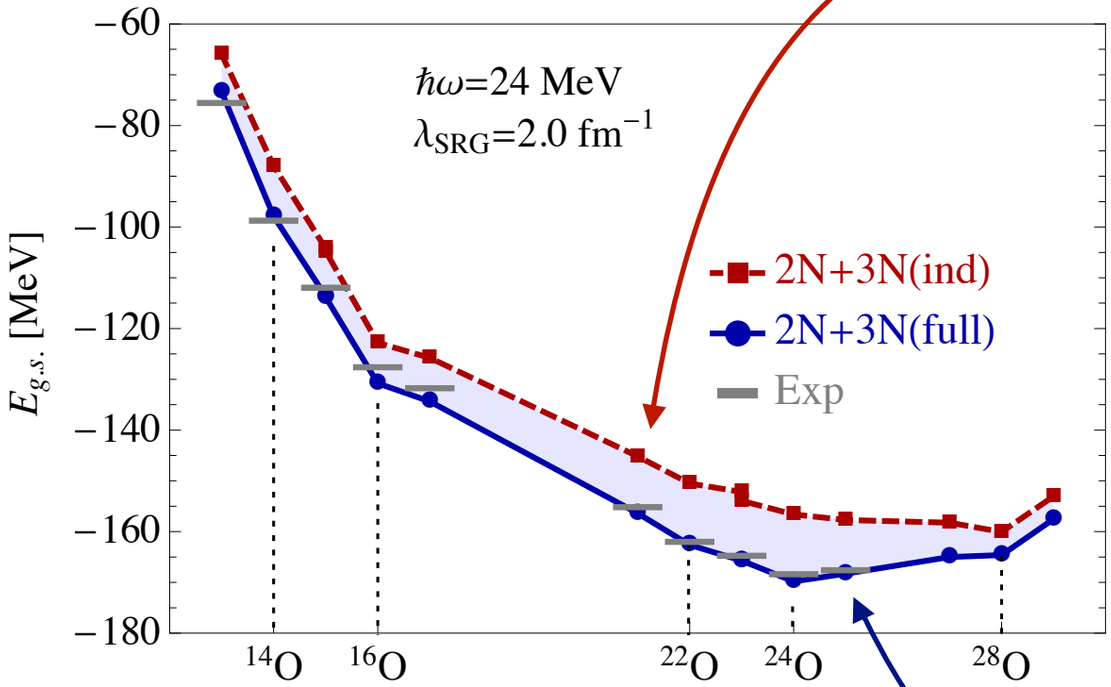


[Cipollone, Barbieri & Navrátil 2013]

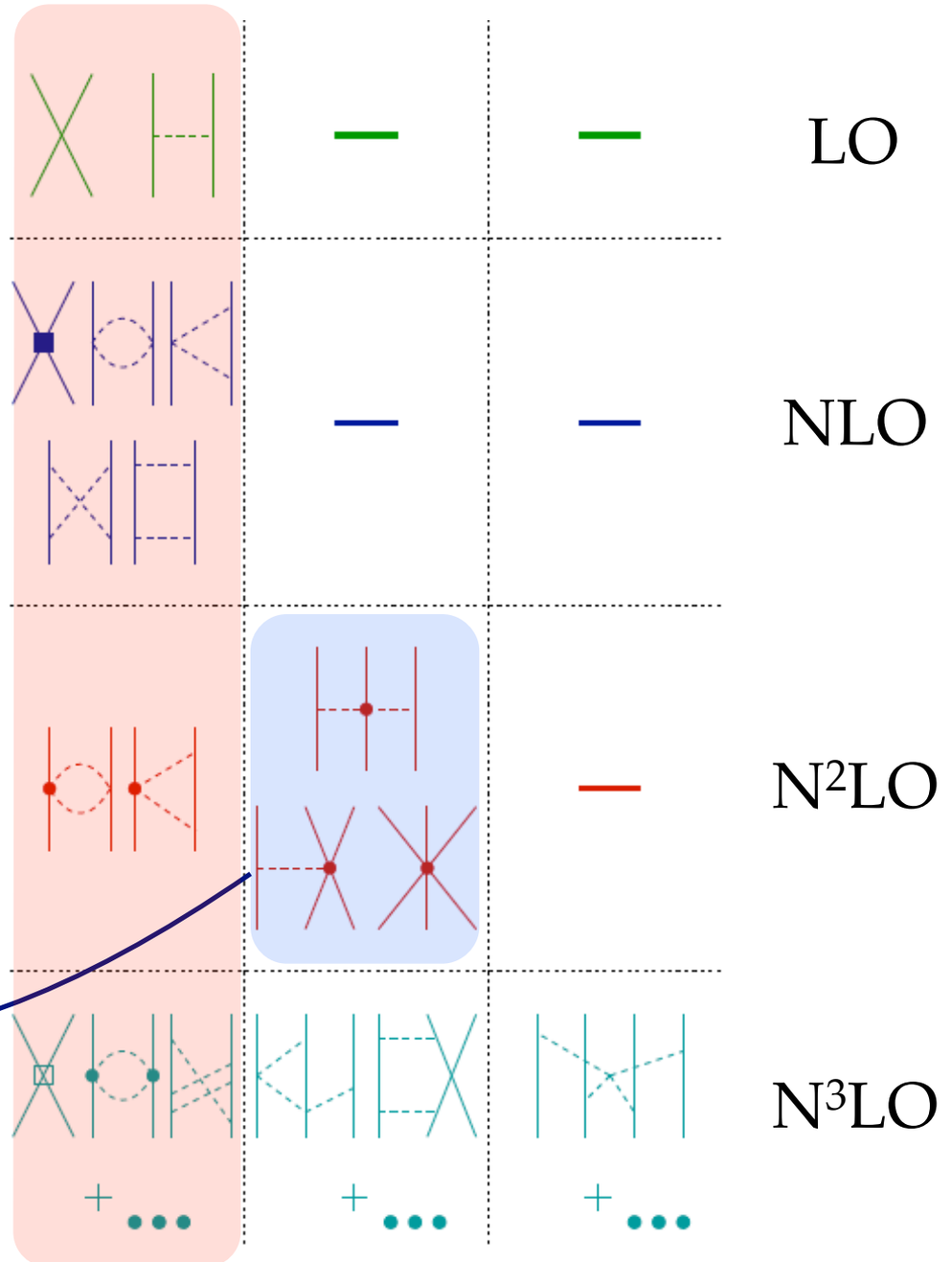


Chiral NN+3N in the oxygen chain

✪ Self-consistent Green's functions



[Cipollone, Barbieri & Navrátil 2013]

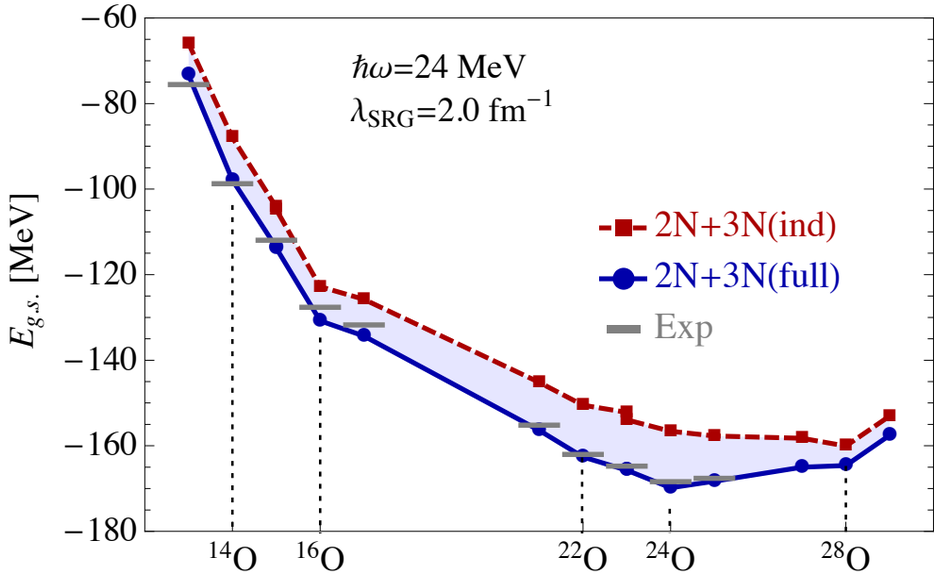


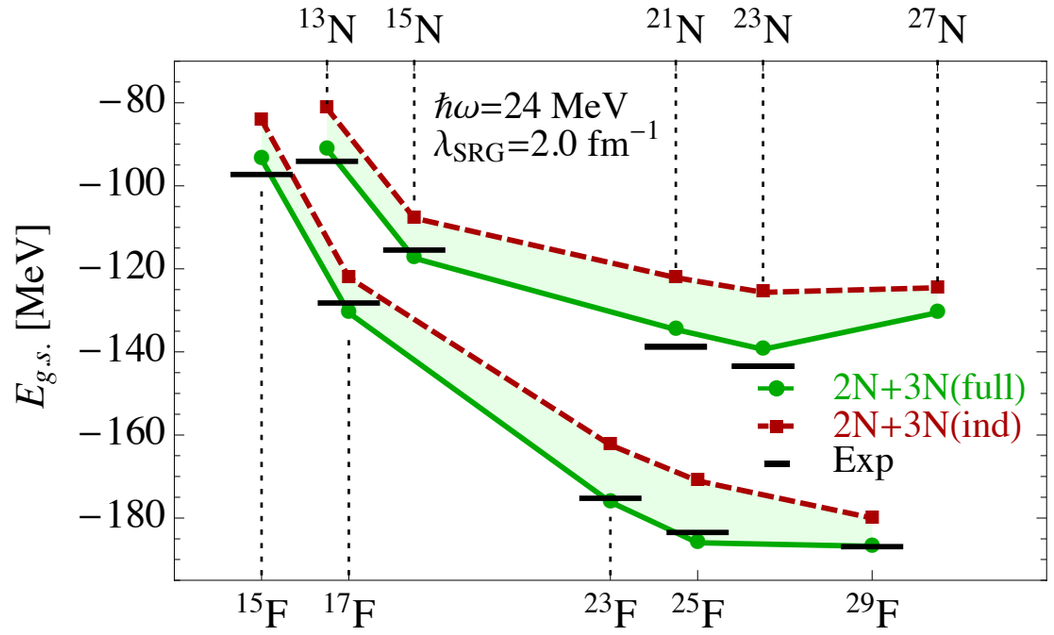
➠ Overall good agreement with data

➠ 3NF crucial for reproducing driplines

Chiral NN+3N in the oxygen chain (and nearby)

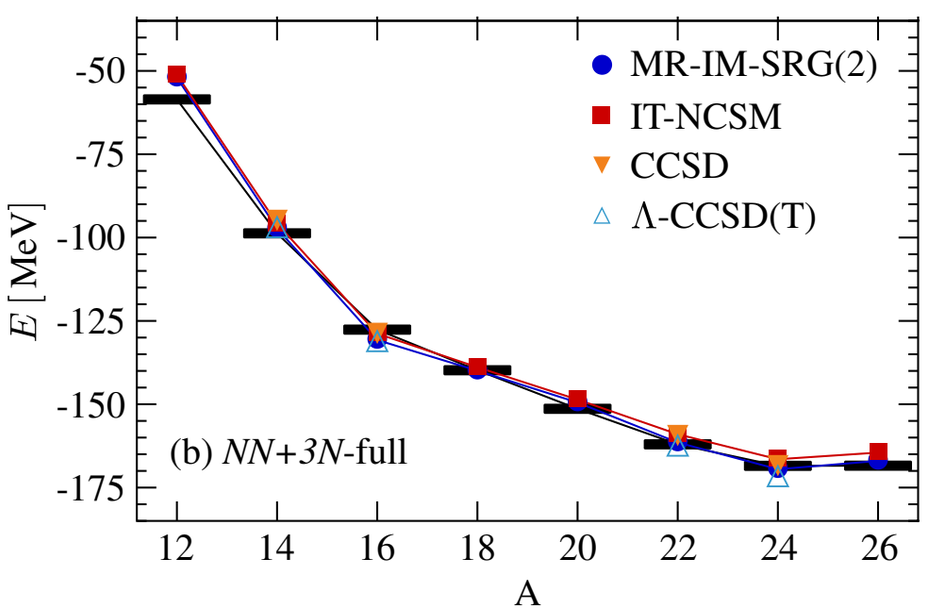
✪ Extend description to Z = 7 and 9 isotopic chains with GF method

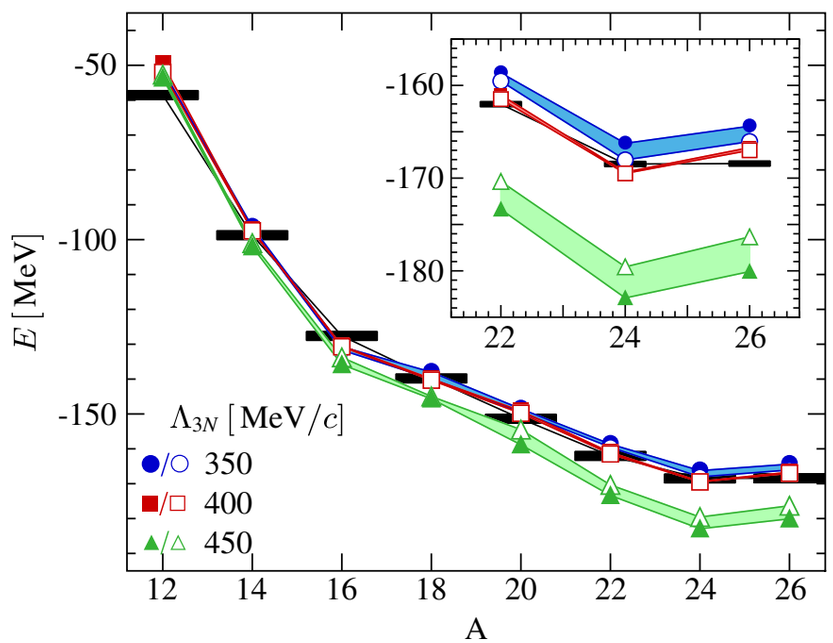




[Cipollone *et al.* 2013]

✪ Excellent agreement between different ab initio methods

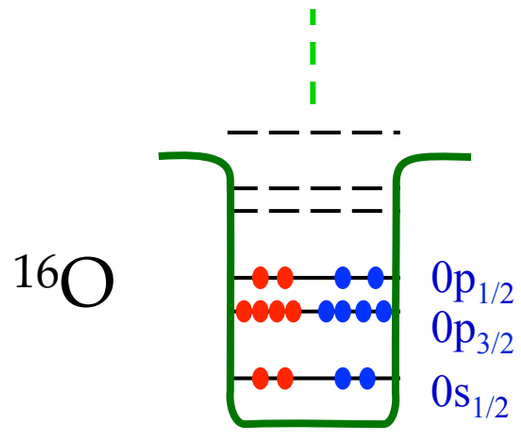




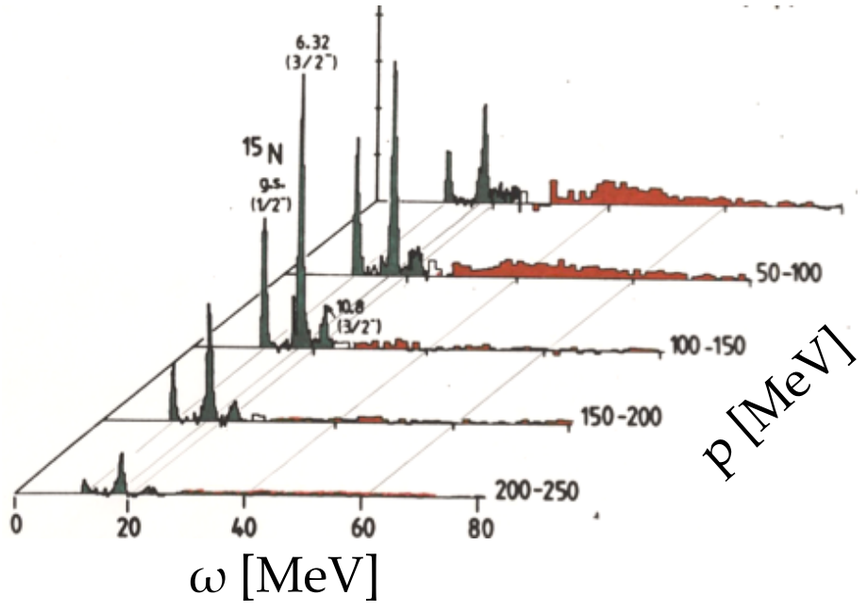
[Hergert *et al.* 2013]

Inside the Green's function

Independent-particle picture



Experiment



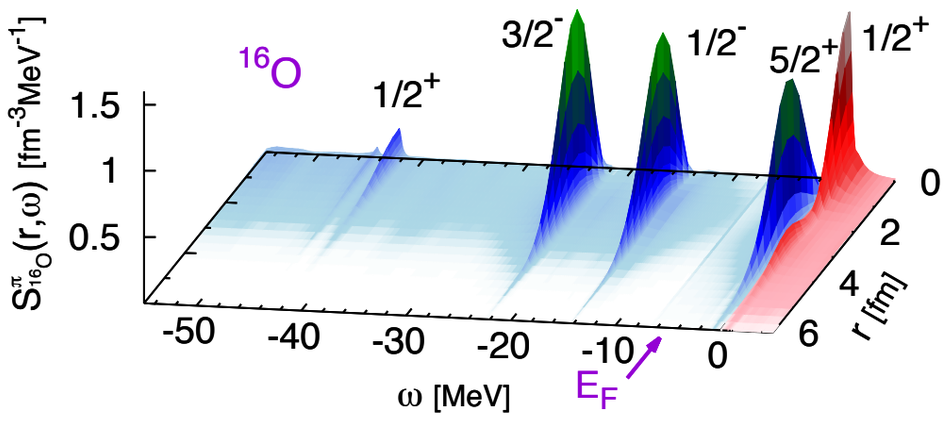
Saclay data for ^{16}O(e,e'p) [Mougey *et al.* 1980]

Green's function calculation

Spectral function

$$S_a^-(\omega) \equiv \sum_k \left|\langle \psi_k^{A-1}|a_a|\psi_0^A\rangle\right|^2 \delta(\omega-(E_0^A-E_k^{A-1})) = \frac{1}{\pi}\mathrm{Im}\, G_{aa}(\omega)$$

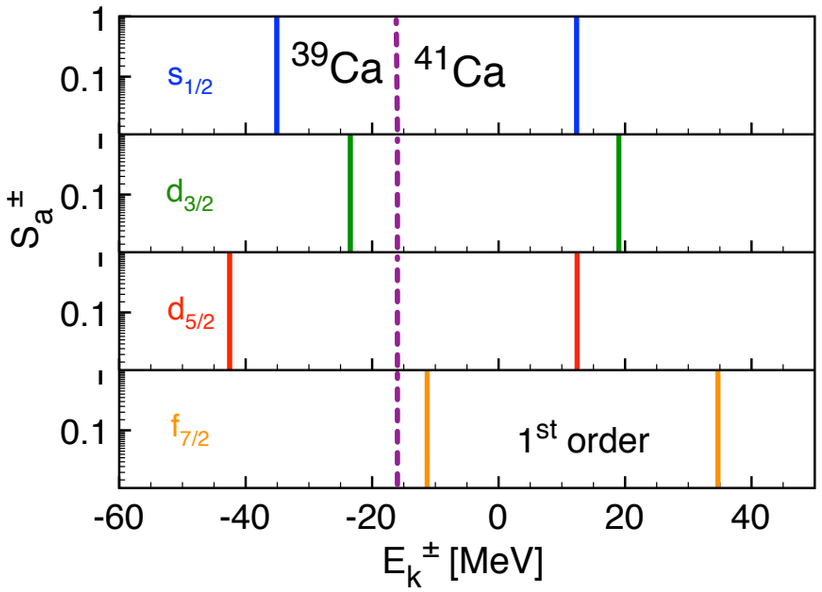
$$S(r,\omega) = \sum_{\alpha\ \beta} \phi_\alpha(\mathbf{r}) \left[S^p_{\alpha\beta}(\omega) + S^h_{\alpha\beta}(\omega)\right] \phi^*_\beta(\mathbf{r})$$



[Cipollone *et al.* 2014]

Spectral strength distribution

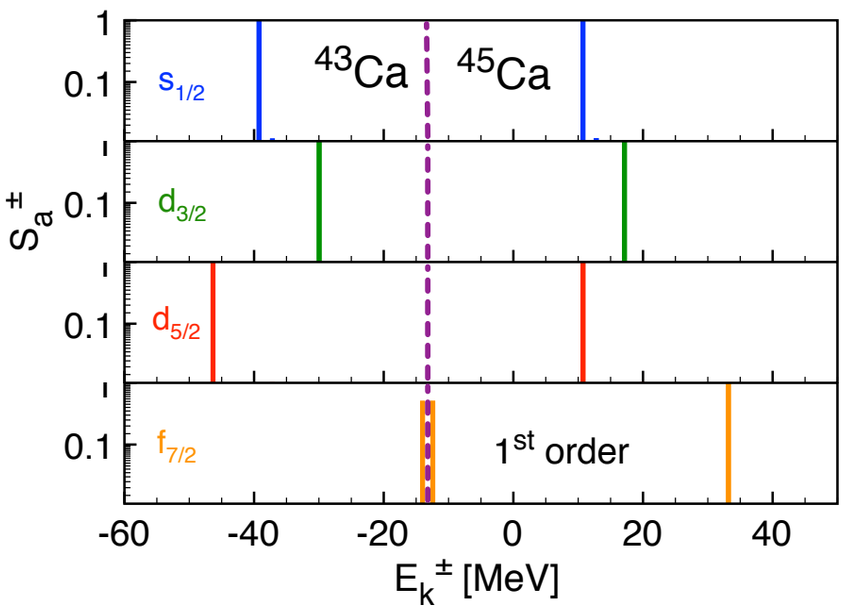
Dyson 1st order (HF)



Fragmentation

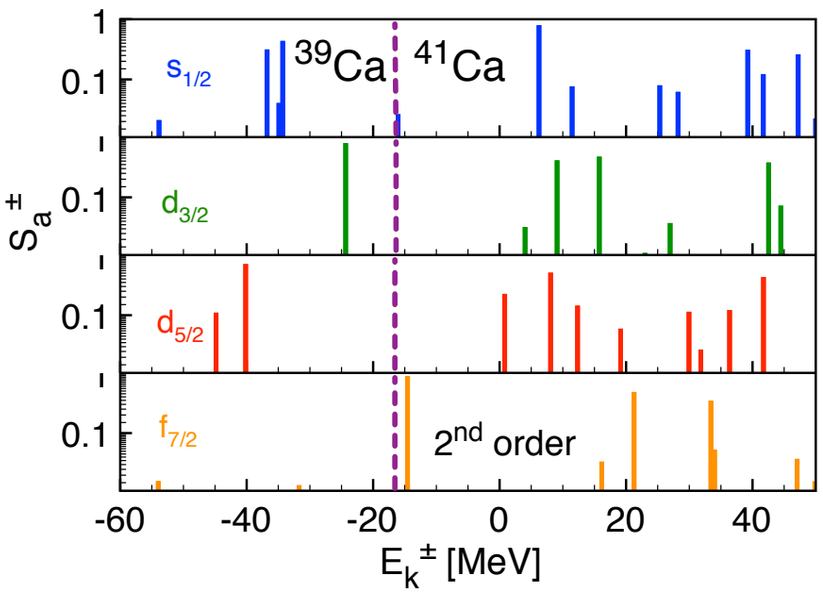
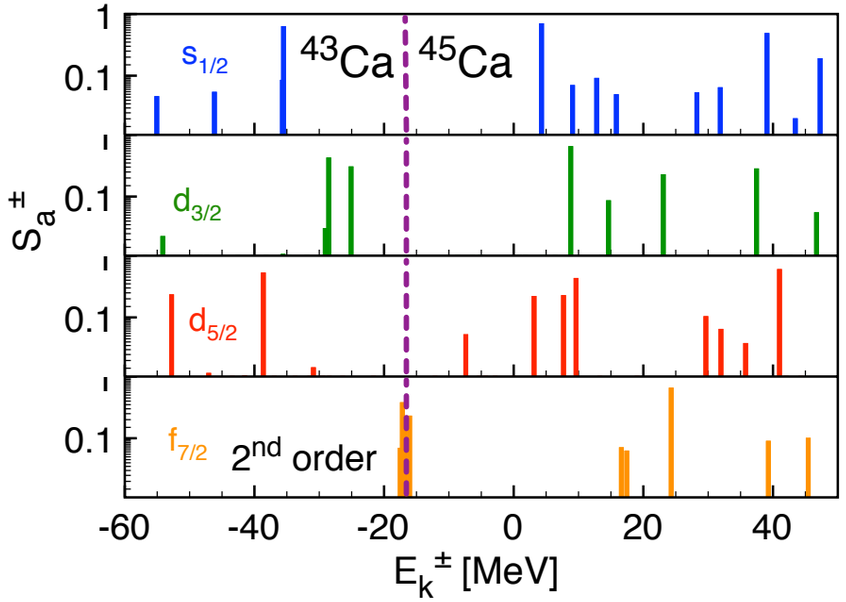
Static pairing

Gorkov 1st order (HFB)



Dynamical fluctuations

Dyson 2nd order



Gorkov 2nd order