Open-shell nuclei from first principles

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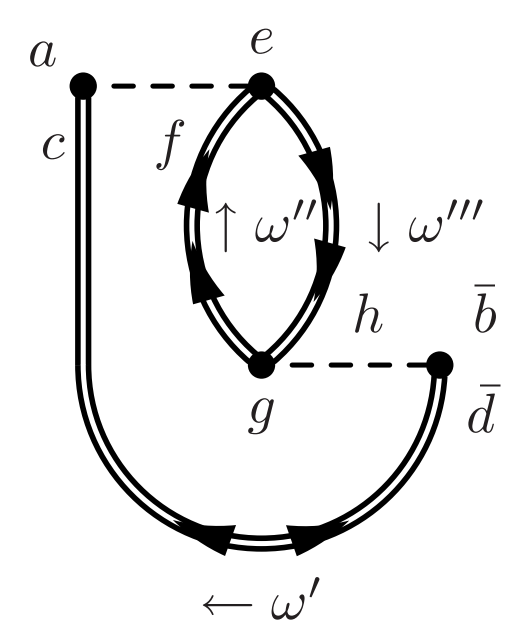

Based on:
VS, Duguet, Barbieri, PRC 84 064317 (2011)
VS, Barbieri, Duguet, arXiv:1208.2472 (2012)

INT program *Light nuclei from first principles*
Seattle, 18 October 2012

Outline

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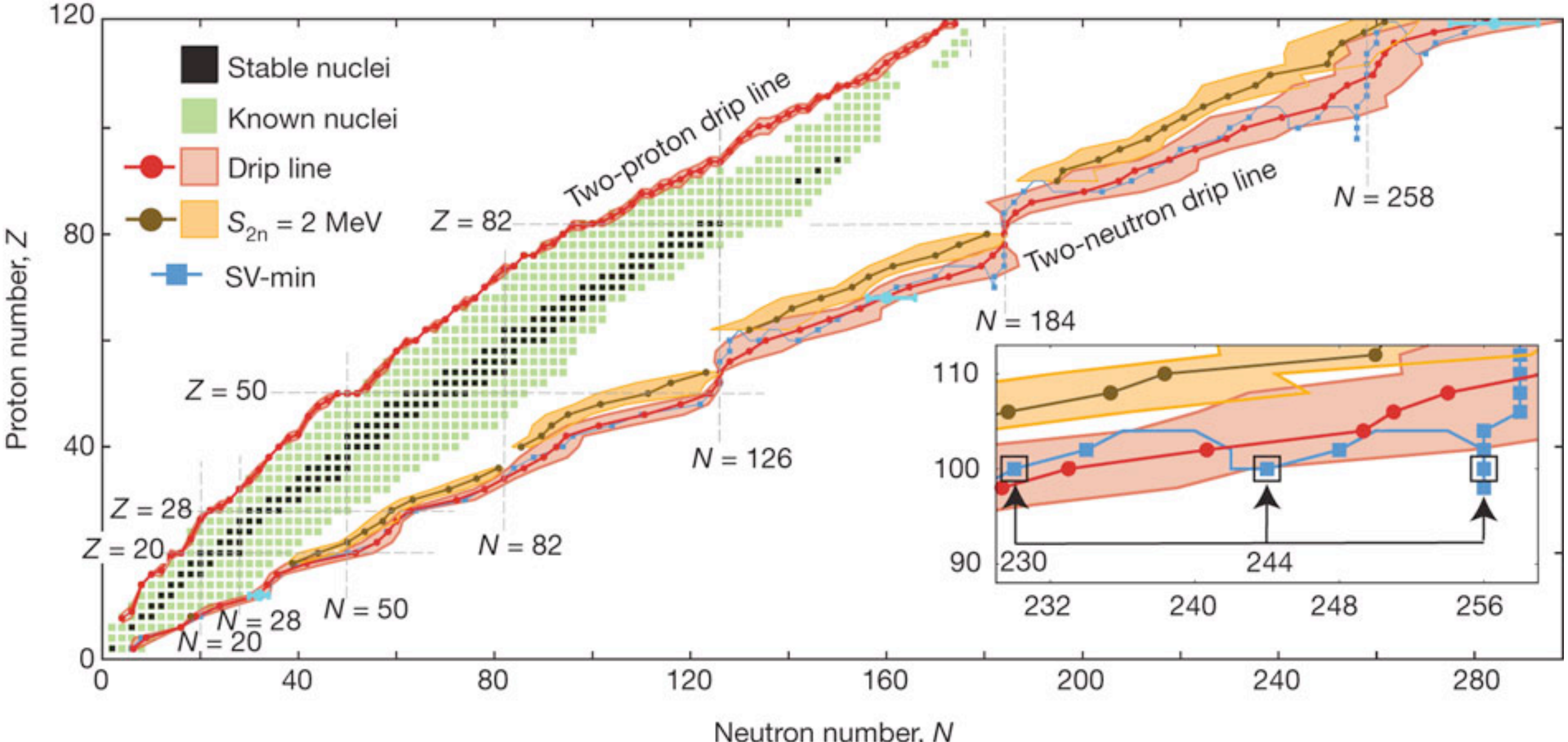
- Introduction
- Gorkov-Green's functions approach
- Results: benchmarks, calcium chain, ^{74}Ni
- Outlook

Introduction

Towards a unified description of nuclei



[Erler *et al.* 2009]

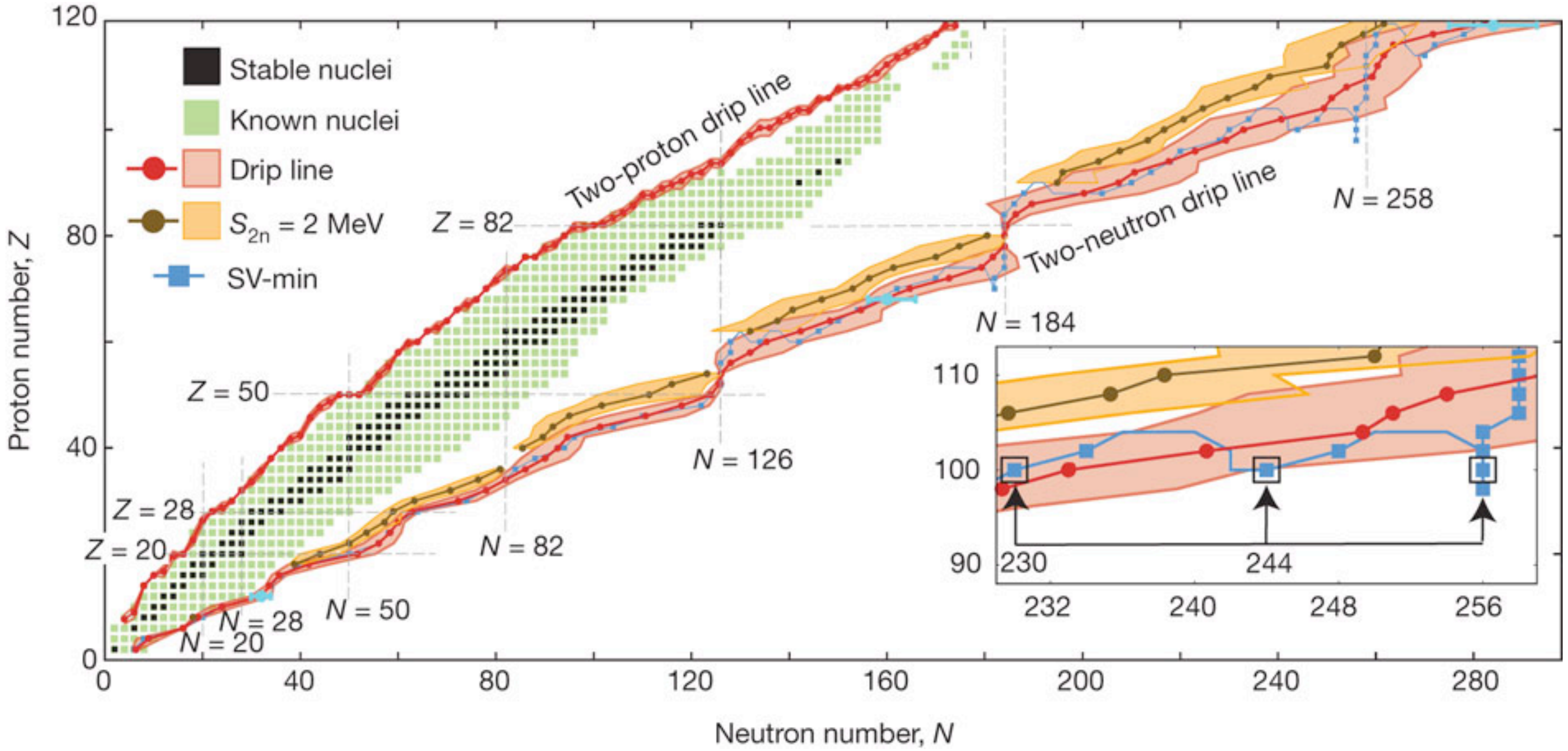
“Exact” methods (NCSM, GFMC, ...)

Ab-initio approaches (CC, SCGF, IM-SRG)

Shell model

SR and MR energy density functionals

Towards a unified description of nuclei



Main challenges:

✔ Good nuclear Hamiltonians

✔ Proper treatment of continuum

✘ Connection to reactions

✘ Extension to open-shell systems

Medium-mass ab-initio nuclear structure

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- Configuration interaction techniques become unfeasible in large spaces
  - ➟ Solution of the nuclear many-body problem has to be approximated

- Ab-initio approaches to medium-mass nuclei
  - ➟ No core, all nucleons active
  - ➟ Only inputs are NN & NNN interactions
  - ➟ Rely on a controlled expansion

- Examples:
  - Self-consistent Dyson-Green's function [Barbieri, Dickhoff, ...]
  - Coupled-cluster [Dean, Hagen, Hjorth-Jensen, Papenbrock, ...]
  - In-medium similarity renormalization group [Bogner, Hergert, Schwenk, Tsukiyama,...]

  ➟ But limited to to doubly-closed-shell ± 1 and ± 2 nuclei

Timeliness of the open-shell endeavor

- Beams of exotic isotopes becoming available worldwide
  - ➠ Predictive theoretical models needed
- Nuclear interactions from chiral EFT
  - ➠ Consistent many-body forces
  - ➠ A way to quantify theoretical errors
- Renormalization group techniques for NN and 3N forces
  - ➠ Many-body problem more perturbative
- Benchmarks for more phenomenological methods
  - ➠ Non-empirical EDF, (microscopic) shell model, ...

Gorkov-Green's function approach

Going open-shell: Gorkov's idea

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- Keep the simplicity of a single-reference

- Address explicitly the non-perturbative formation of Cooper pairs

  ➡ Formulate the expansion scheme around a Bogoliubov vacuum

  ➡ Breaking of particle-number conservation (eventually restored)

- Auxiliary many-body state

  ➡ Mixes various particle numbers $|\Psi_0\rangle \equiv \sum_{A}^{\text{even}} c_A \, |\psi_0^A\rangle$

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

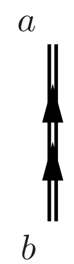
  ➡ $|\Psi_0\rangle$ minimizes $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$ under the constraint $A = \langle \Psi_0 | A | \Psi_0 \rangle$

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

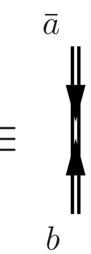
Gorkov equations

✺ Set of 4 Green's functions

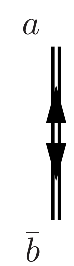
$$i\,G^{11}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{a_a(t)a^\dagger_b(t')\right\}|\Psi_0\rangle \equiv$$



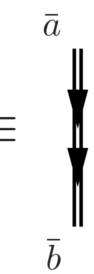
$$i\,G^{21}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{\bar{a}^\dagger_a(t)a^\dagger_b(t')\right\}|\Psi_0\rangle \equiv$$



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



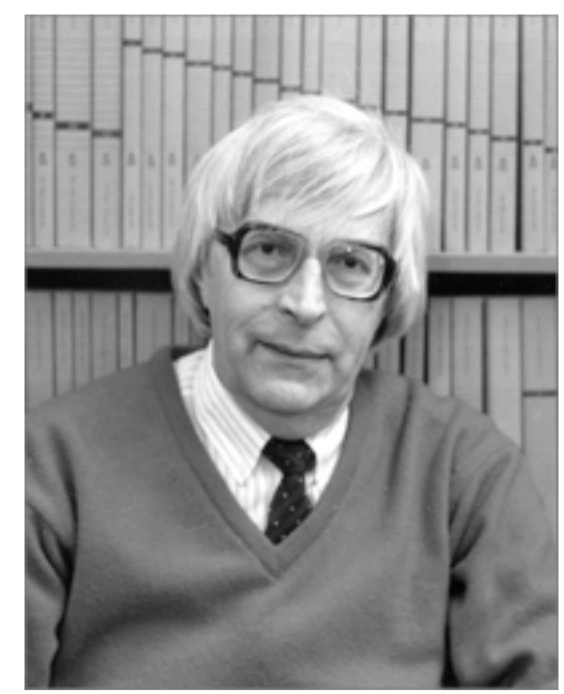
$$i\,G^{22}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{\bar{a}^\dagger_a(t)\bar{a}_b(t')\right\}|\Psi_0\rangle \equiv$$



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

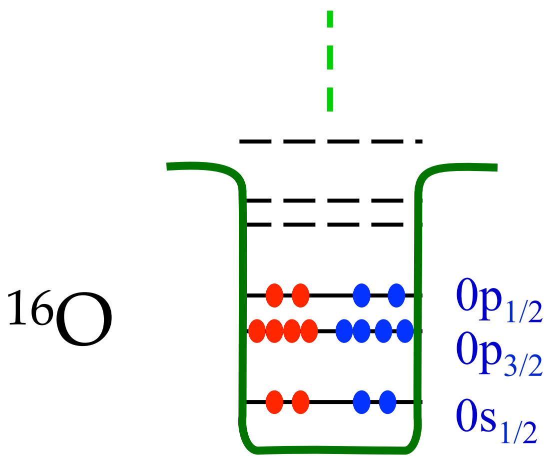
Gorkov equations

[Gorkov 1958]

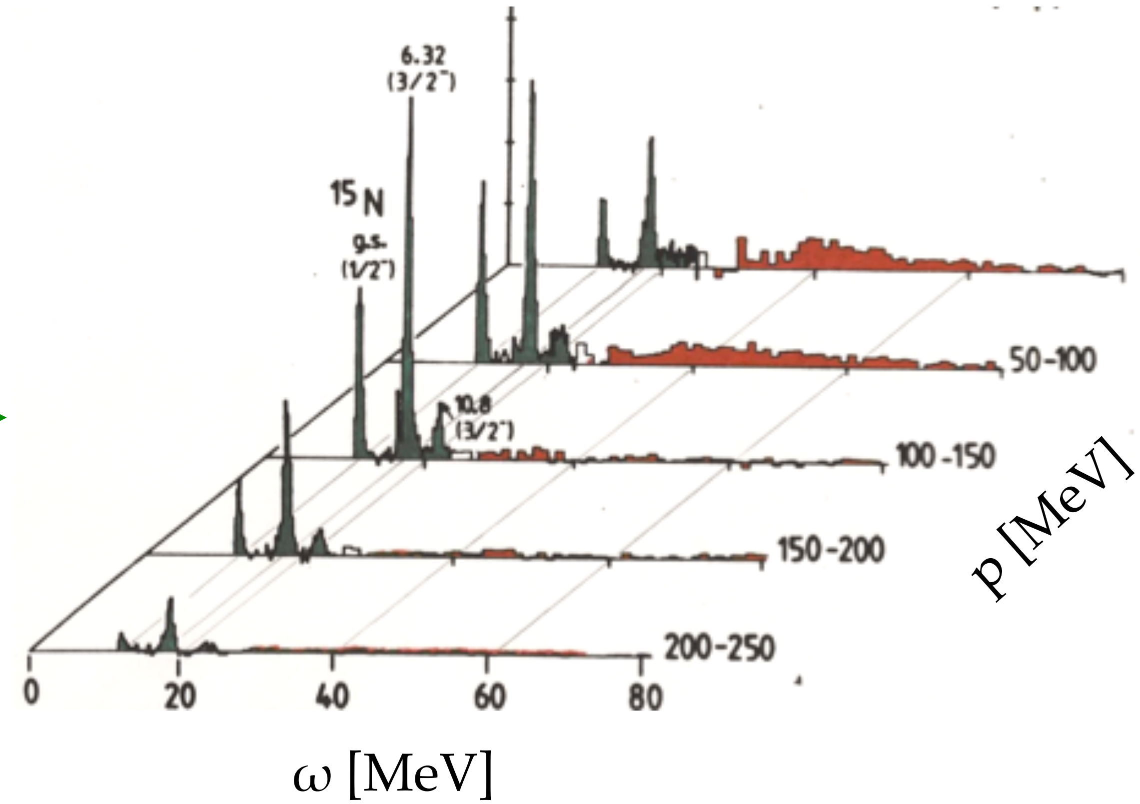


One-nucleon spectral function

✷ Independent-particle picture



correlations →



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

✷ Spectral function

$$S_p^-(\omega) \equiv \sum_k \left|\langle\psi_k^{A-1}|a_p|\psi_0^A\rangle\right|^2 \delta(\omega - (E_0^A - E_k^{A-1}))$$

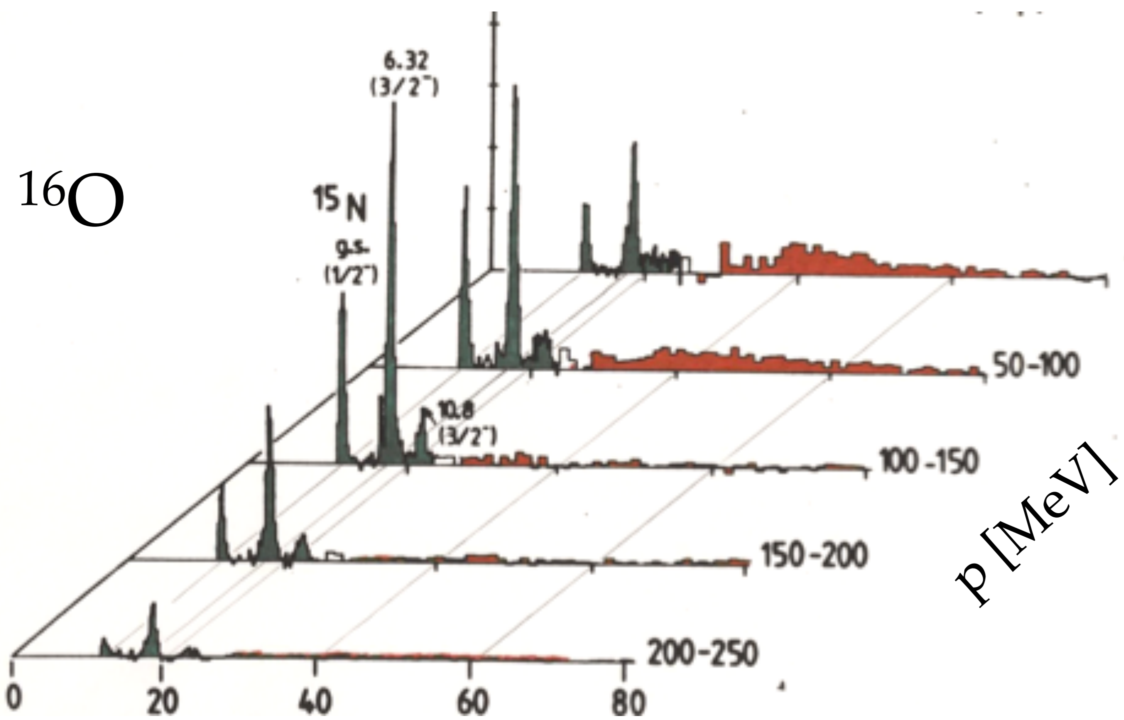
➟ distribution of momenta and energies

One-nucleon Green's function

- Spectral function

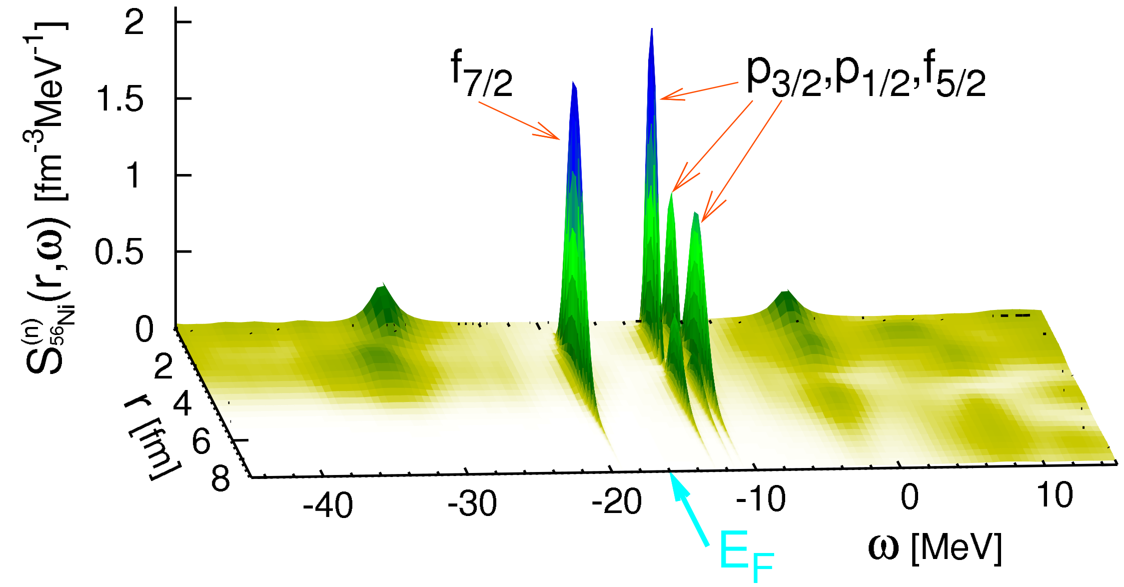
$$S_a^-(\omega) \equiv \sum_k \left|\langle\psi_k^{A-1}|a_a|\psi_0^A\rangle\right|^2 \delta(\omega-(E_0^A-E_k^{A-1})) = \frac{1}{\pi}\mathrm{Im}\,G_{aa}(\omega)$$

^{16}O



ω [MeV]

^{56}Ni



[Barbieri 2009]

One-nucleon Green's function

✺ Spectral function

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

✺ Green's function

$$G_{ab}(\omega) = \sum_k \frac{\langle\psi_0^A|a_a|\psi_k^{A+1}\rangle\langle\psi_k^{A+1}|a_a^\dagger|\psi_0^A\rangle}{\omega-(E_k^{A+1}-E_0^A)+i\eta} + \sum_k \frac{\langle\psi_0^A|a_a^\dagger|\psi_k^{A-1}\rangle\langle\psi_k^{A-1}|a_a|\psi_0^A\rangle}{\omega-(E_0^A-E_k^{A-1})-i\eta}$$

➟ Contains all structure information probed by nucleon transfer

➟ Gives access to:

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

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

Spectrum and spectroscopic factors

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

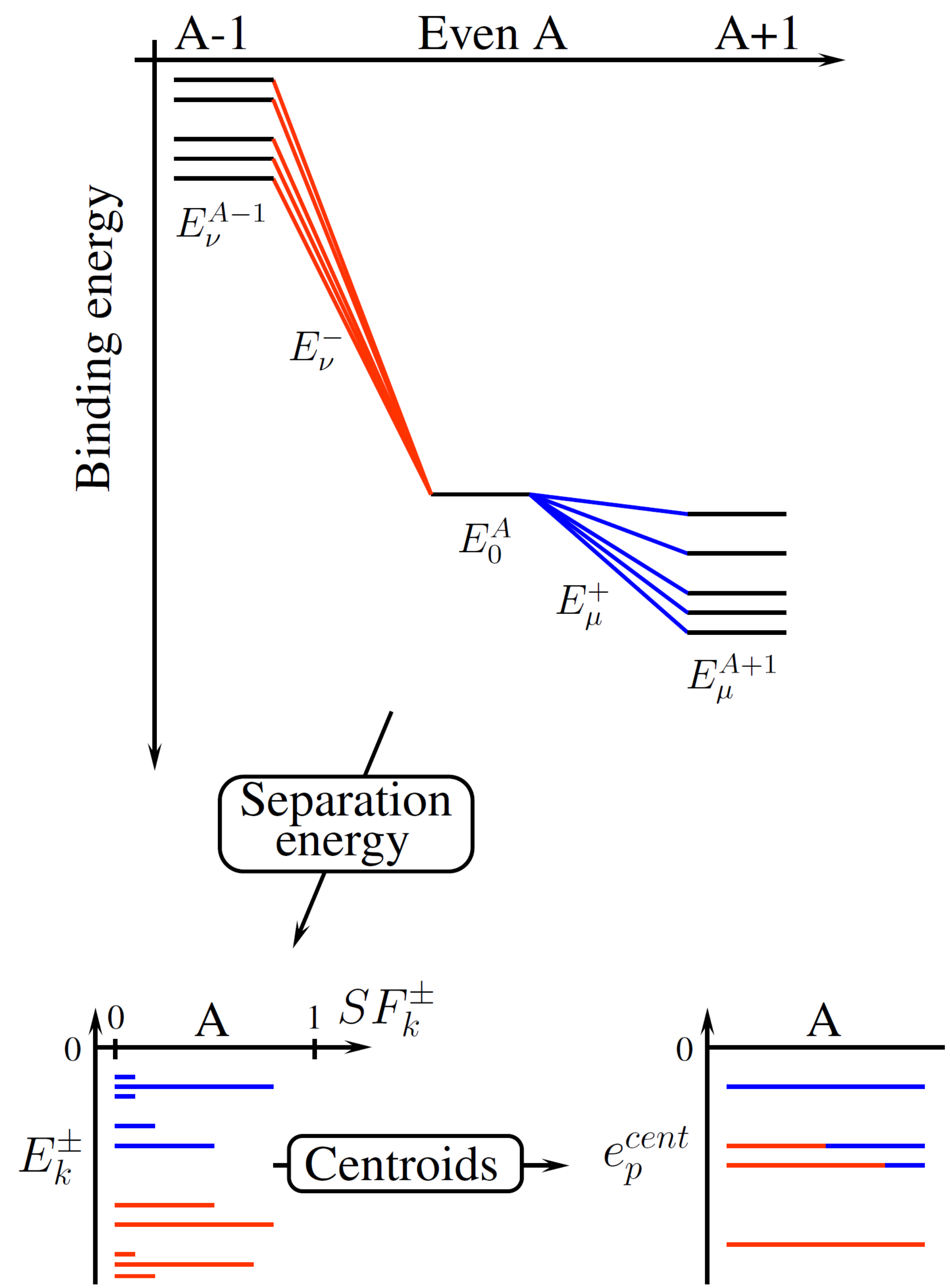
where
$$\begin{cases} \mathcal{U}^{k*}_a \equiv \langle \Psi_k | a^\dagger_a | \Psi_0 \rangle \\ \mathcal{V}^{k*}_a \equiv \langle \Psi_k | \bar{a}_a | \Psi_0 \rangle \end{cases}$$

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

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

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

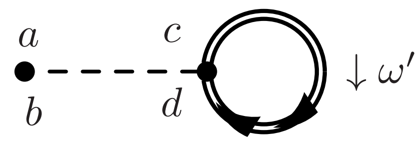


[figure from Sadoudi]

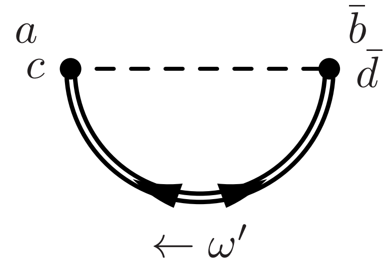
Self-energy truncation

- 1^{st} order ➟ energy-independent self-energy

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

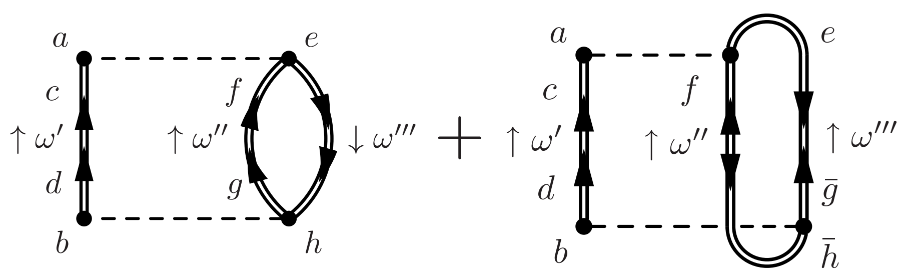


$\Sigma^{12\,(1)}_{ab} =$

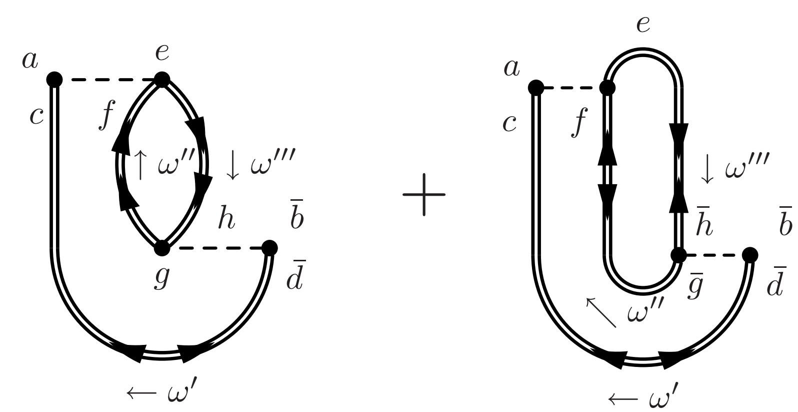


- 2^{nd} order ➟ energy-dependent self-energy

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



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



- Gorkov equations ⟶ energy *dependent* eigenvalue problem

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

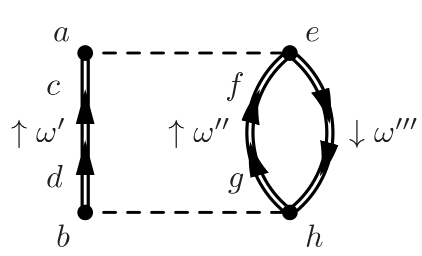
$$\mathcal{U}^{k*}_a \equiv \langle \Psi_k | \bar{a}^\dagger_a | \Psi_0 \rangle$$
$$\mathcal{V}^{k*}_a \equiv \langle \Psi_k | a_a | \Psi_0 \rangle$$

Scaling of Gorkov's problem

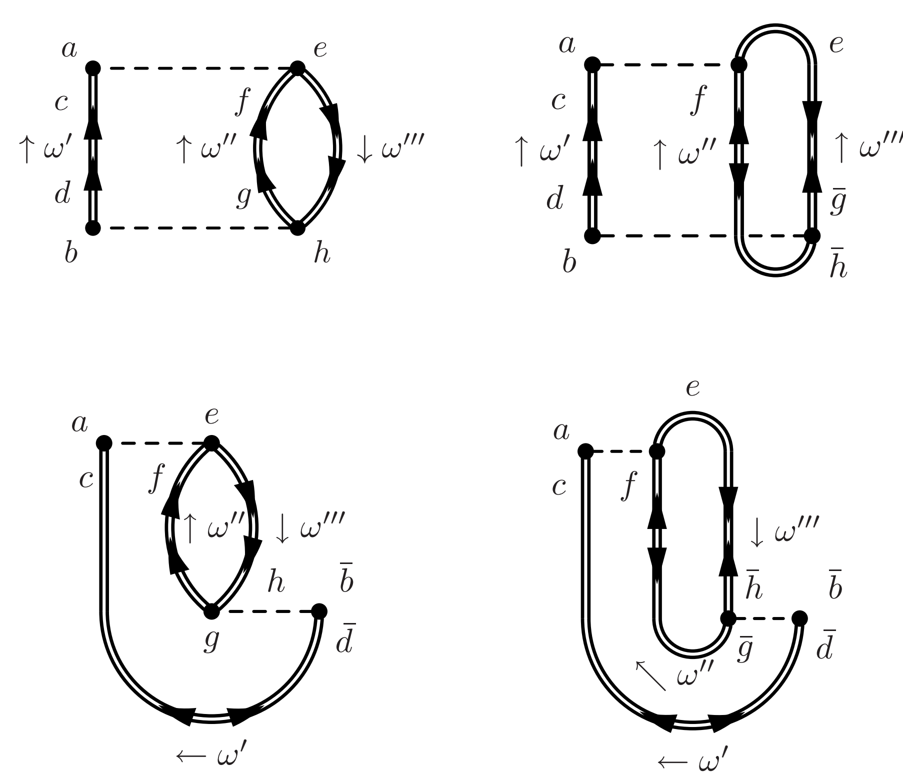
- Transformed into an energy *independent* eigenvalue problem

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

Coupling to 2p1h / 2h1p



Coupling to 3qp



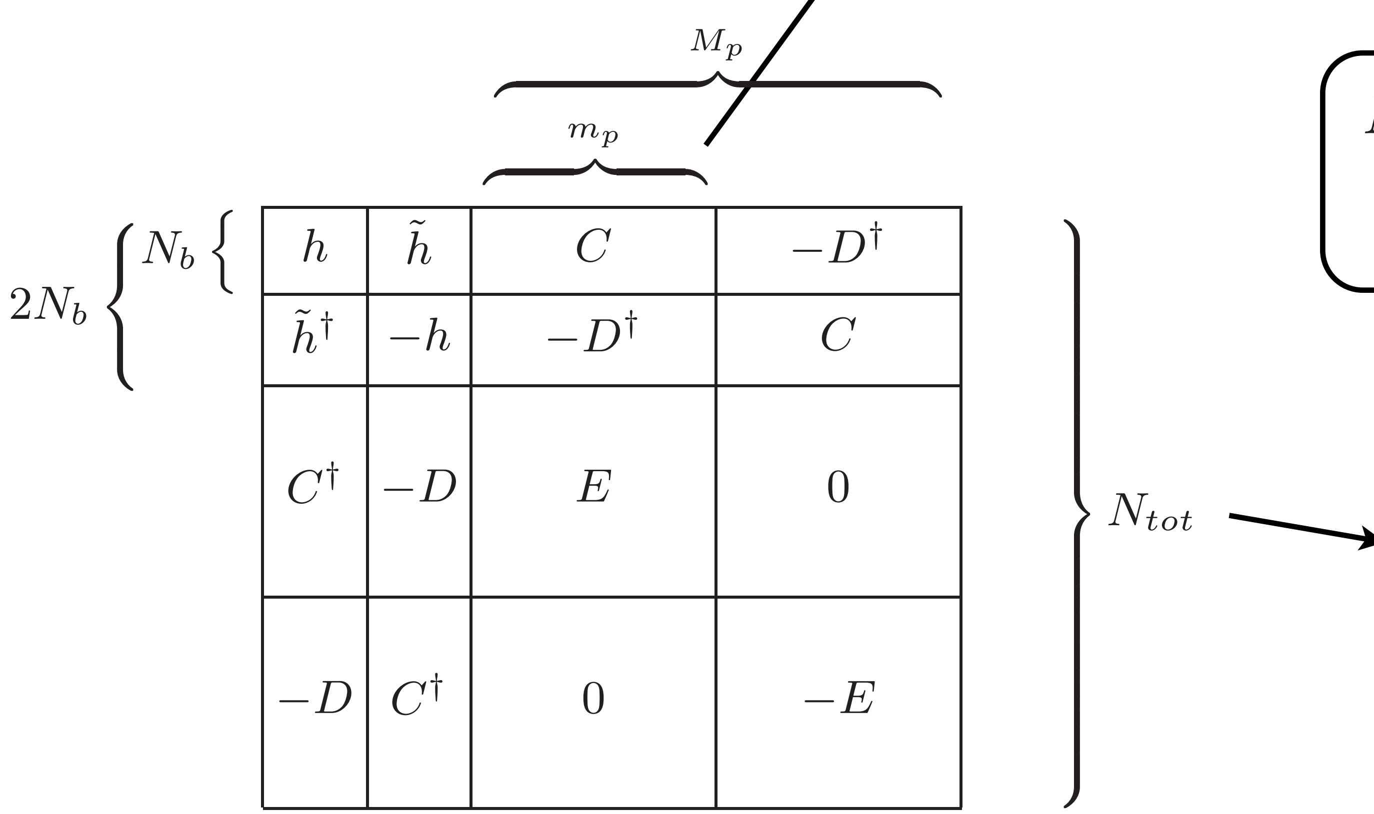
Scaling of Gorkov's problem

- Transformed into an energy *independent* eigenvalue problem

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

- Numerical scaling

$$m_{p,1} \approx \binom{N_b}{3} \propto \frac{N_b^3}{6}$$



N_b → dimension of the s.p. basis

n → number of iterations

$$N_{tot,1} = 2N_b + M_{p,1} \approx N_b^3$$

...

$$N_{tot,n} = 2N_b + M_{p,n} \approx N_b^{3n}$$

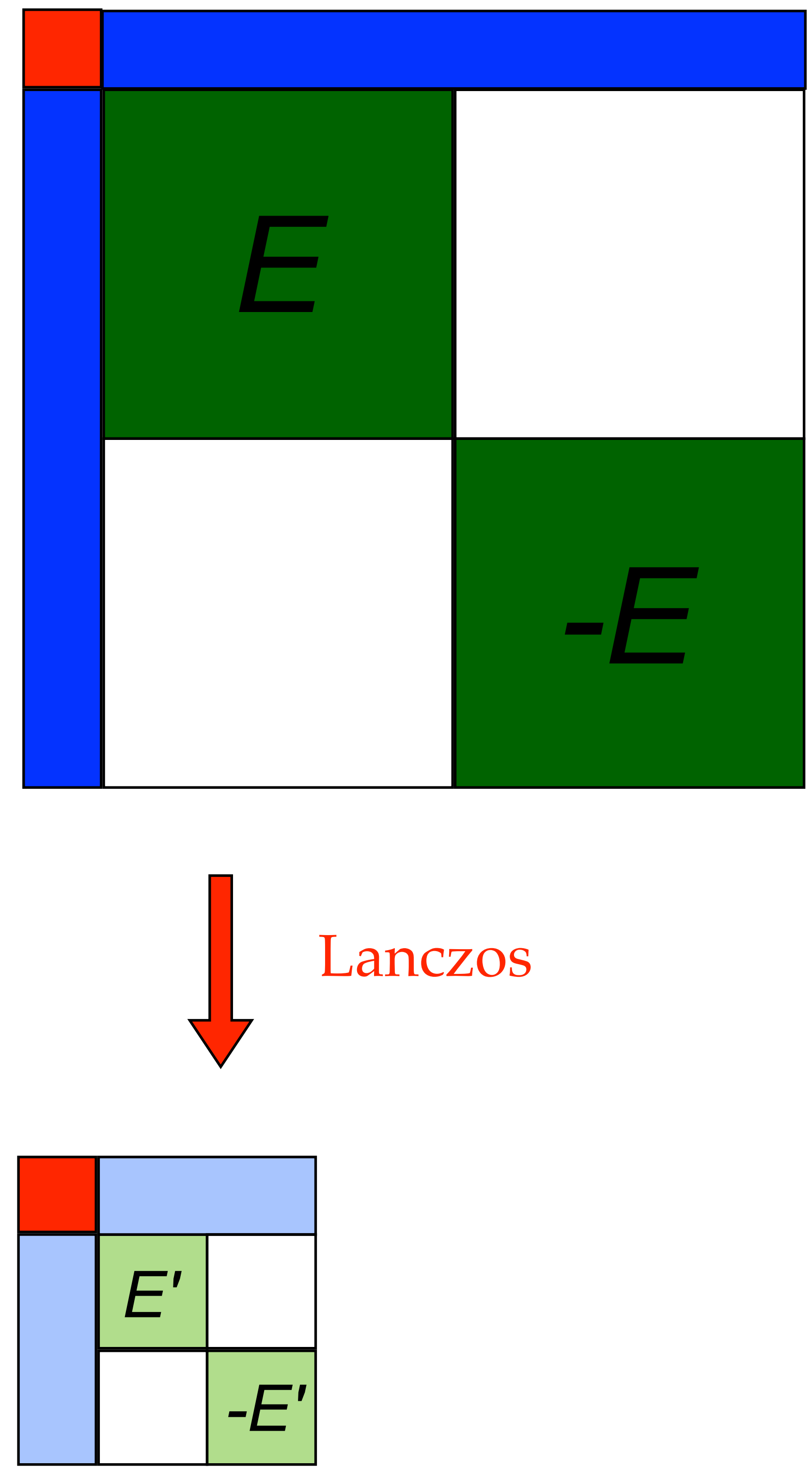
Tame the dimension growth

How do we select the poles?

We do not...

Instead, Lanczos projection of Gorkov matrix

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



➠ Conserves moments of spectral functions

➠ Equivalent to exact diagonalization for $N_L \to \dim(E)$

Test Lanczos projection

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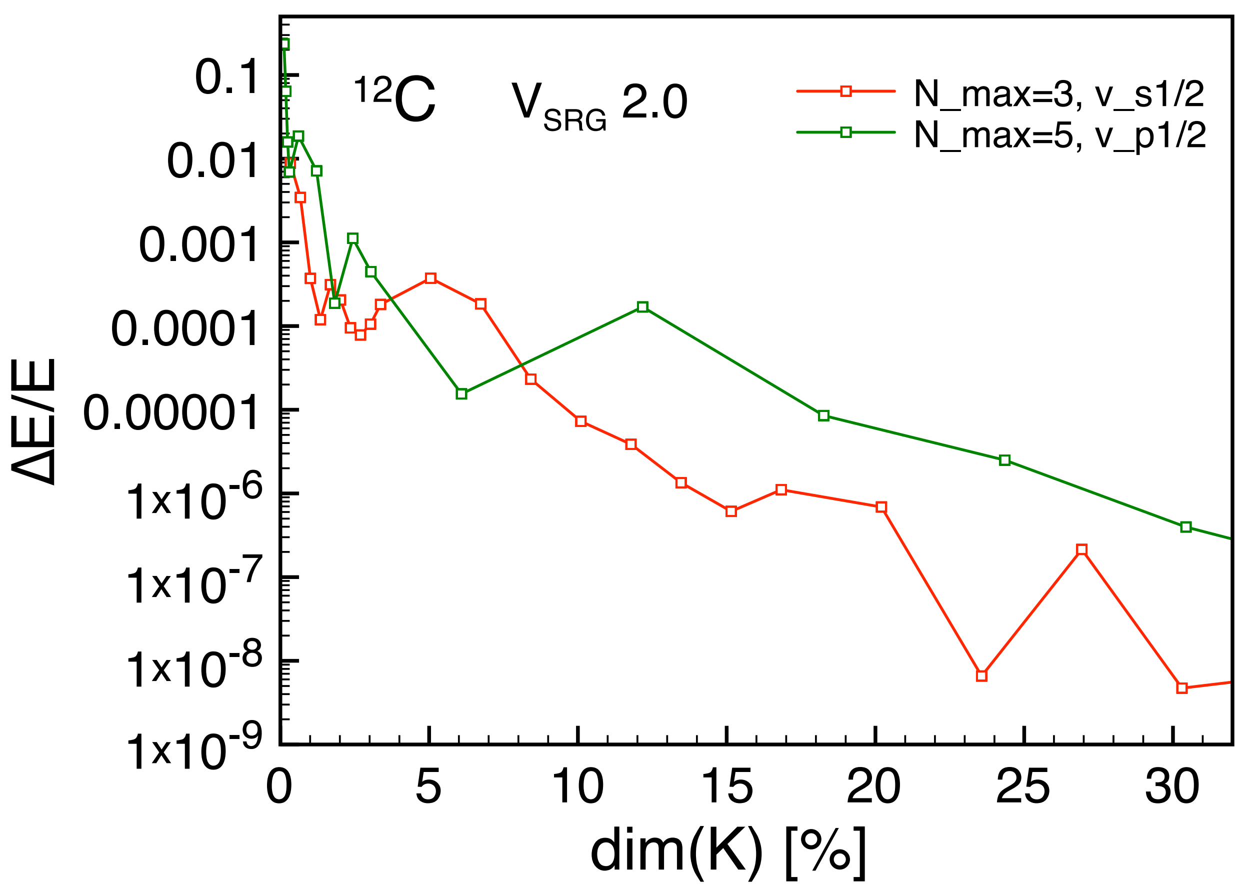
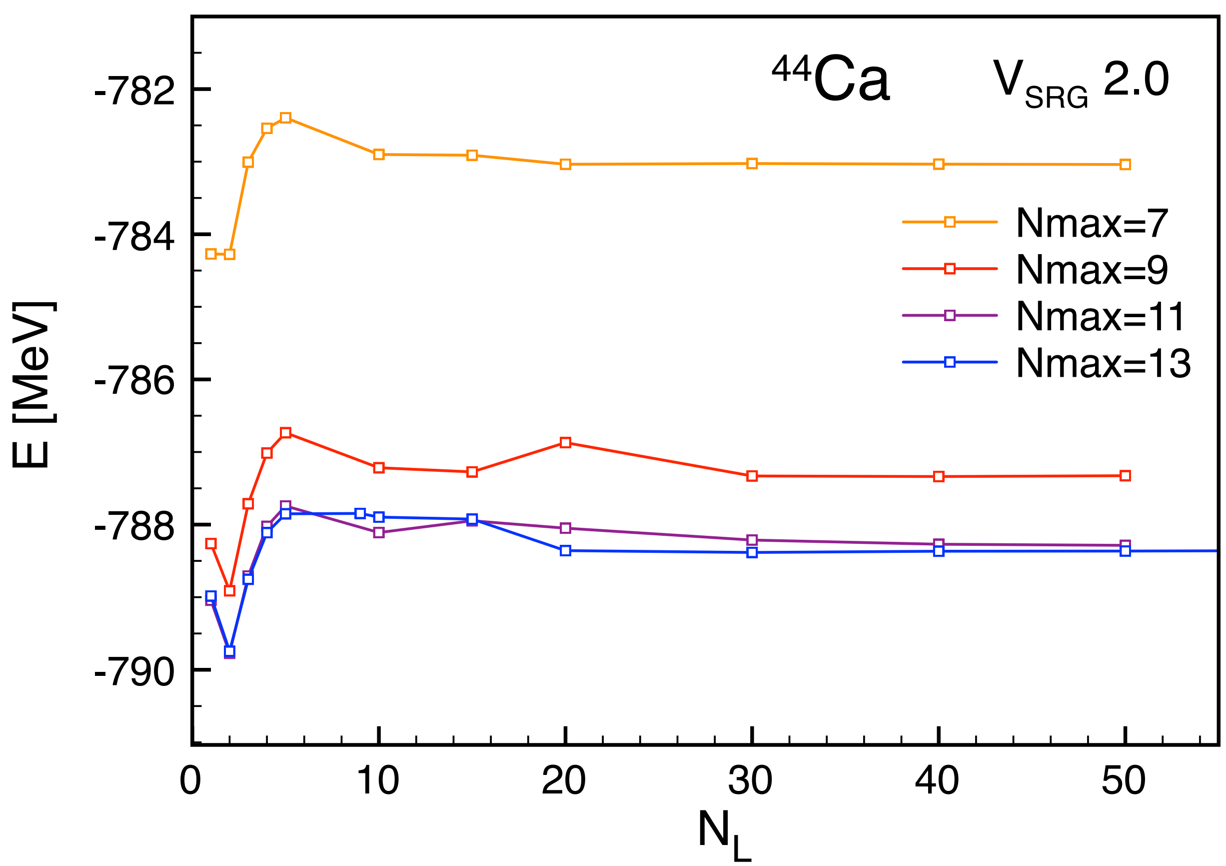
One diagonalization



Self-consistent



➟ Good convergence towards exact digonalization

Results

Benchmark with coupled cluster method

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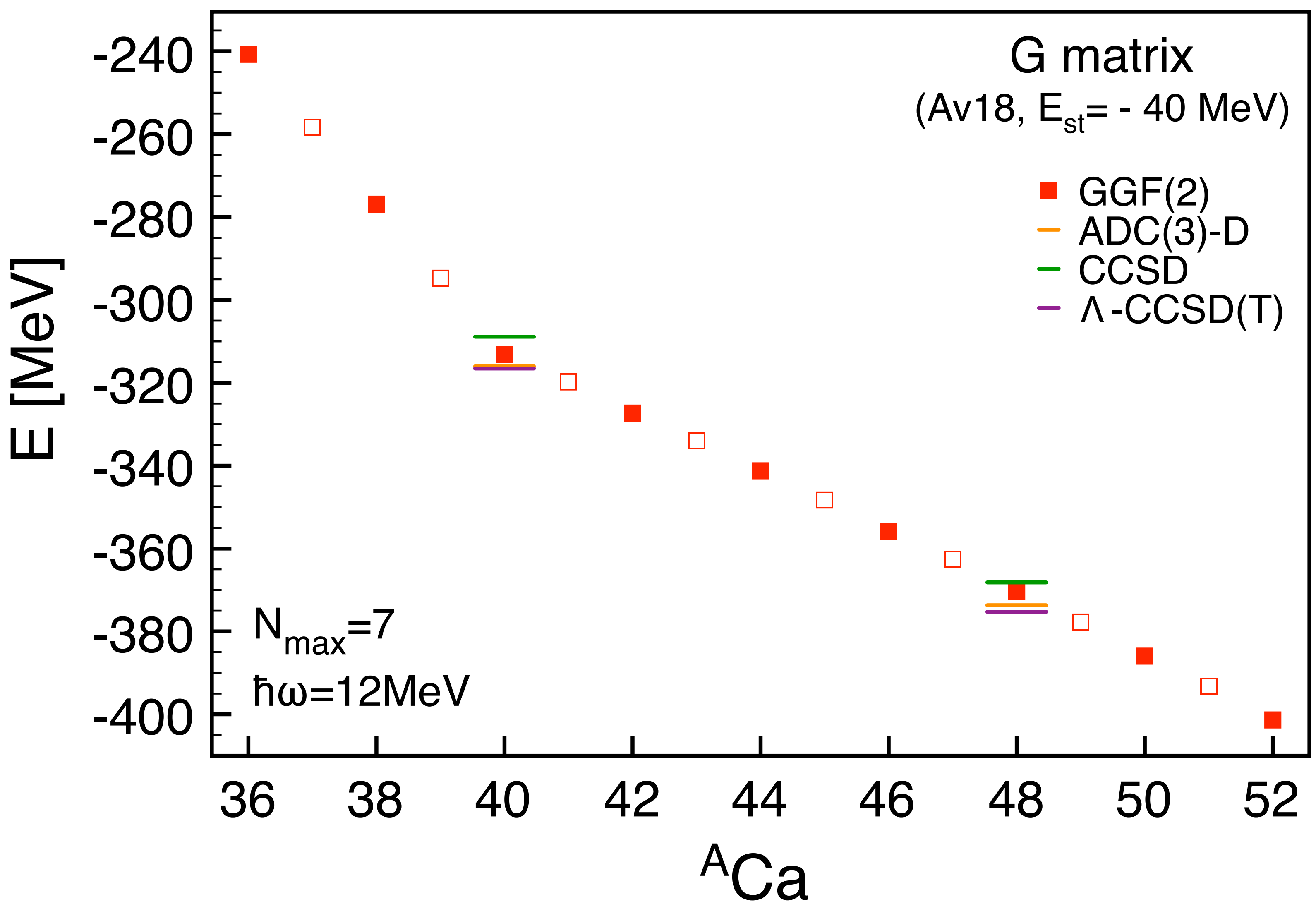

➟ GGF and CC quantitatively similar

➟ GGF(3) expected to reach Λ-CCSD(T) accuracy

(CC results courtesy of G. Hagen)

Spectral strength distribution

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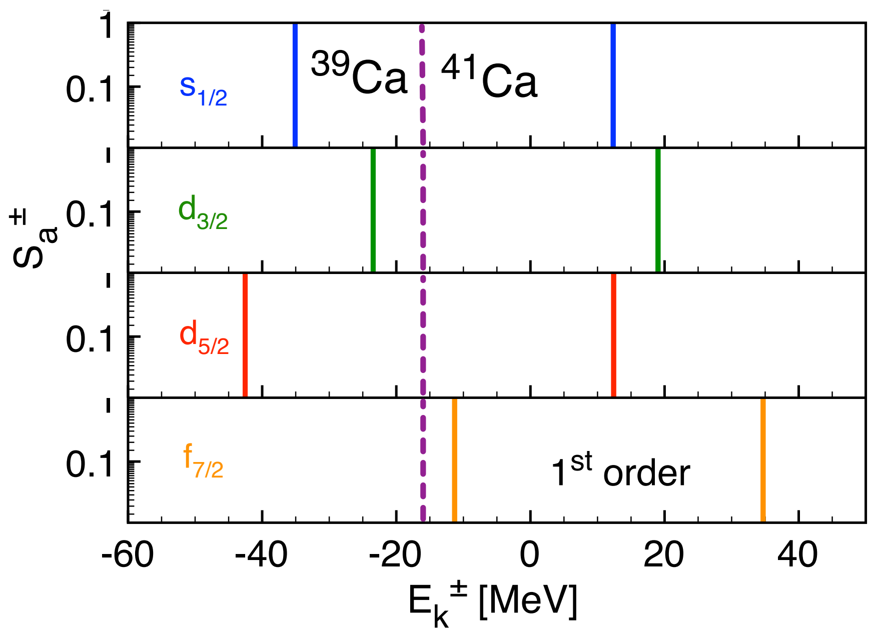
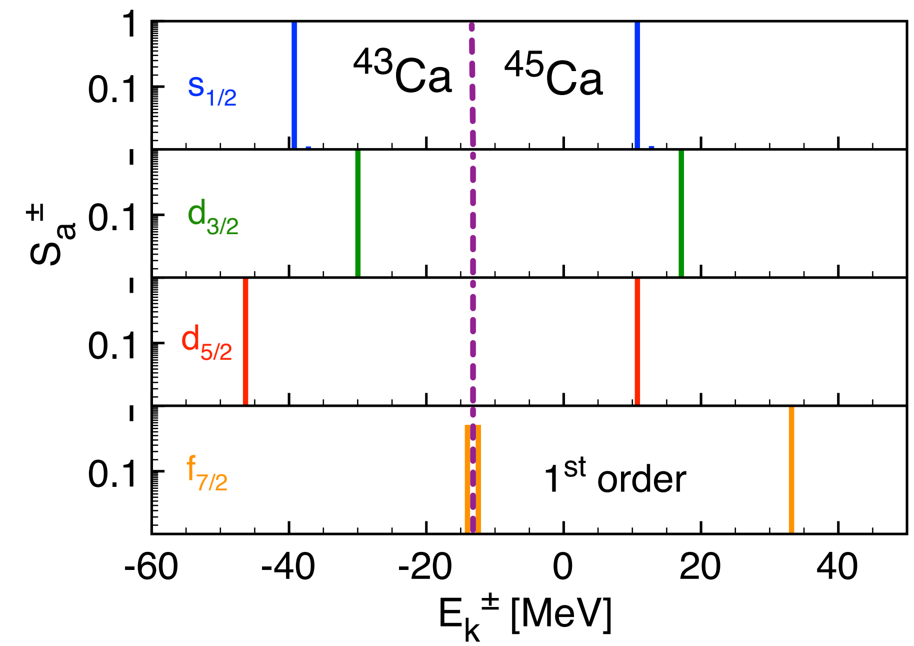
Dyson 1st order (HF)



Fragmentation

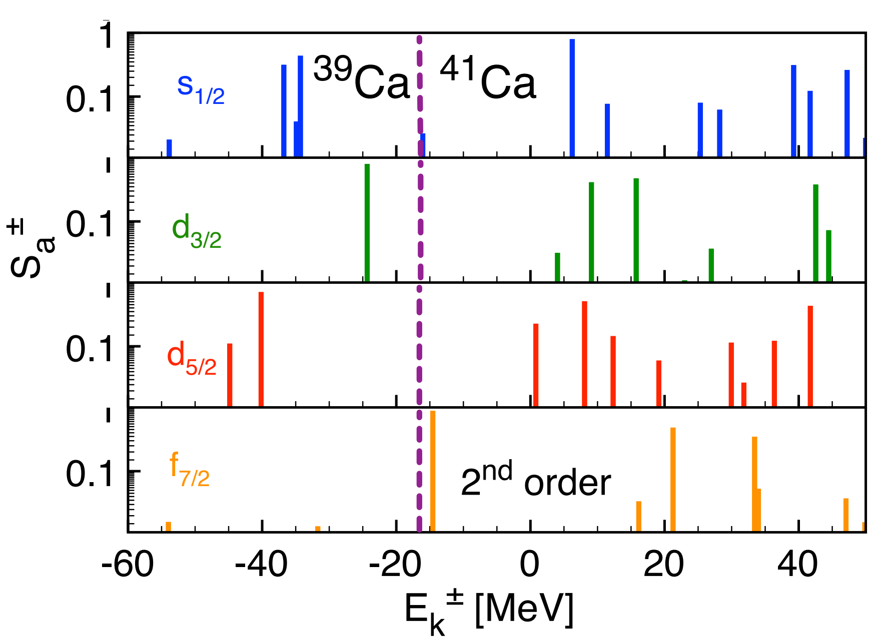
Static pairing

Gorkov 1st order (HFB)

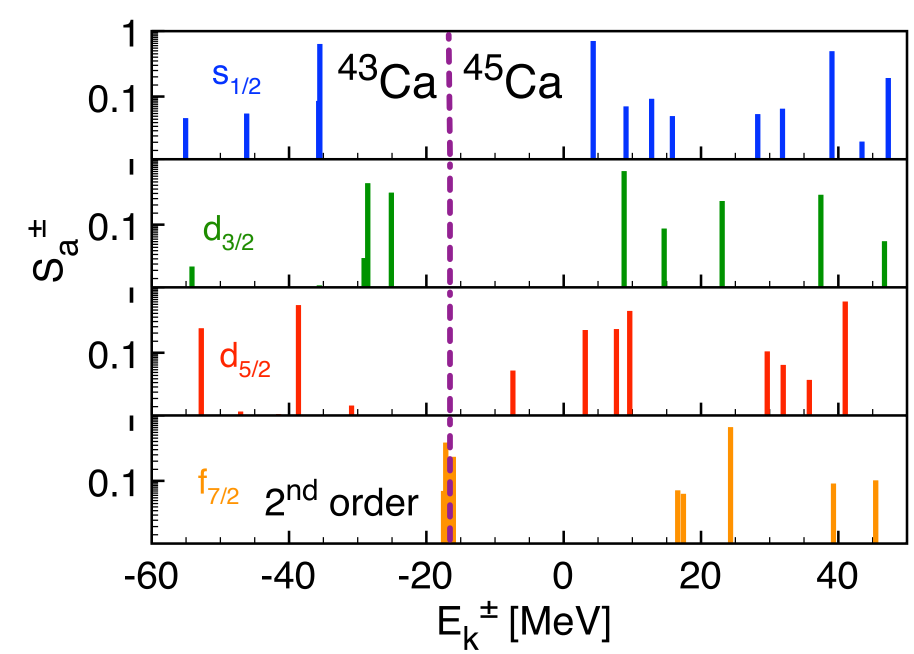


Dynamical fluctuations

Dyson 2nd order



Gorkov 2nd order



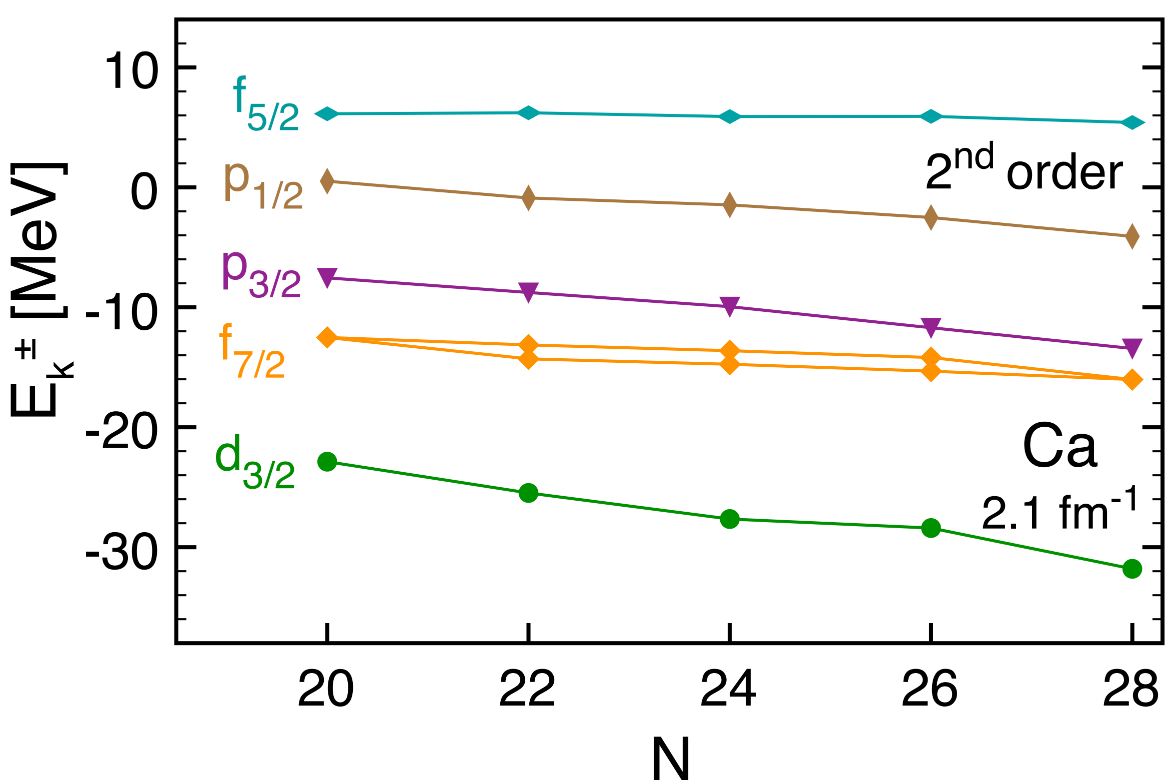
Shell structure evolution

✺ ESPE collect fragmentation of "single-particle" strengths from both N±1

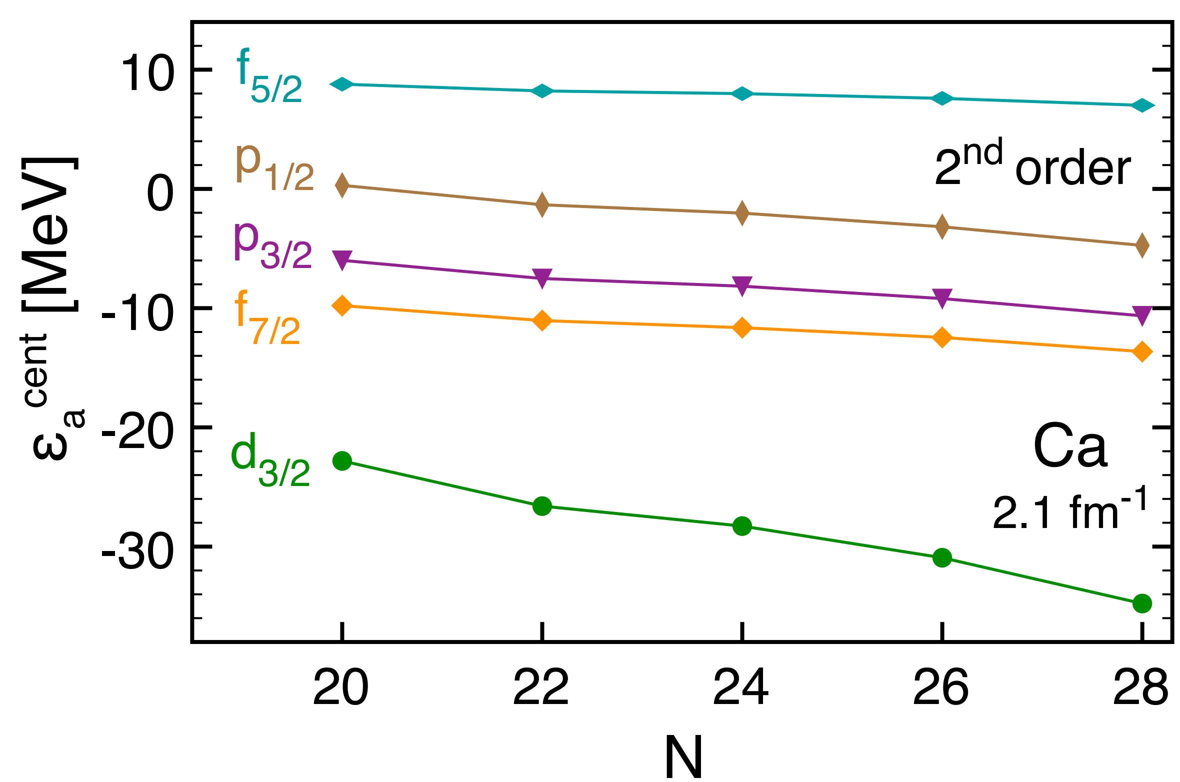
$$\epsilon_a^{cent} \equiv h_{ab}^{cent}\,\delta_{ab} = t_{aa} + \sum_{cd} \bar{V}_{acad}^{NN}\,\rho_{dc}^{[1]} + \sum_{cdef} \bar{V}_{acdaef}^{NNN}\,\rho_{efcd}^{[2]} \equiv \sum_k \mathcal{S}_k^{+a} E_k^{+} + \sum_k \mathcal{S}_k^{-a} E_k^{-}$$

[Baranger 1970, Duguet and Hagen. 2011]

Quasiparticle peaks

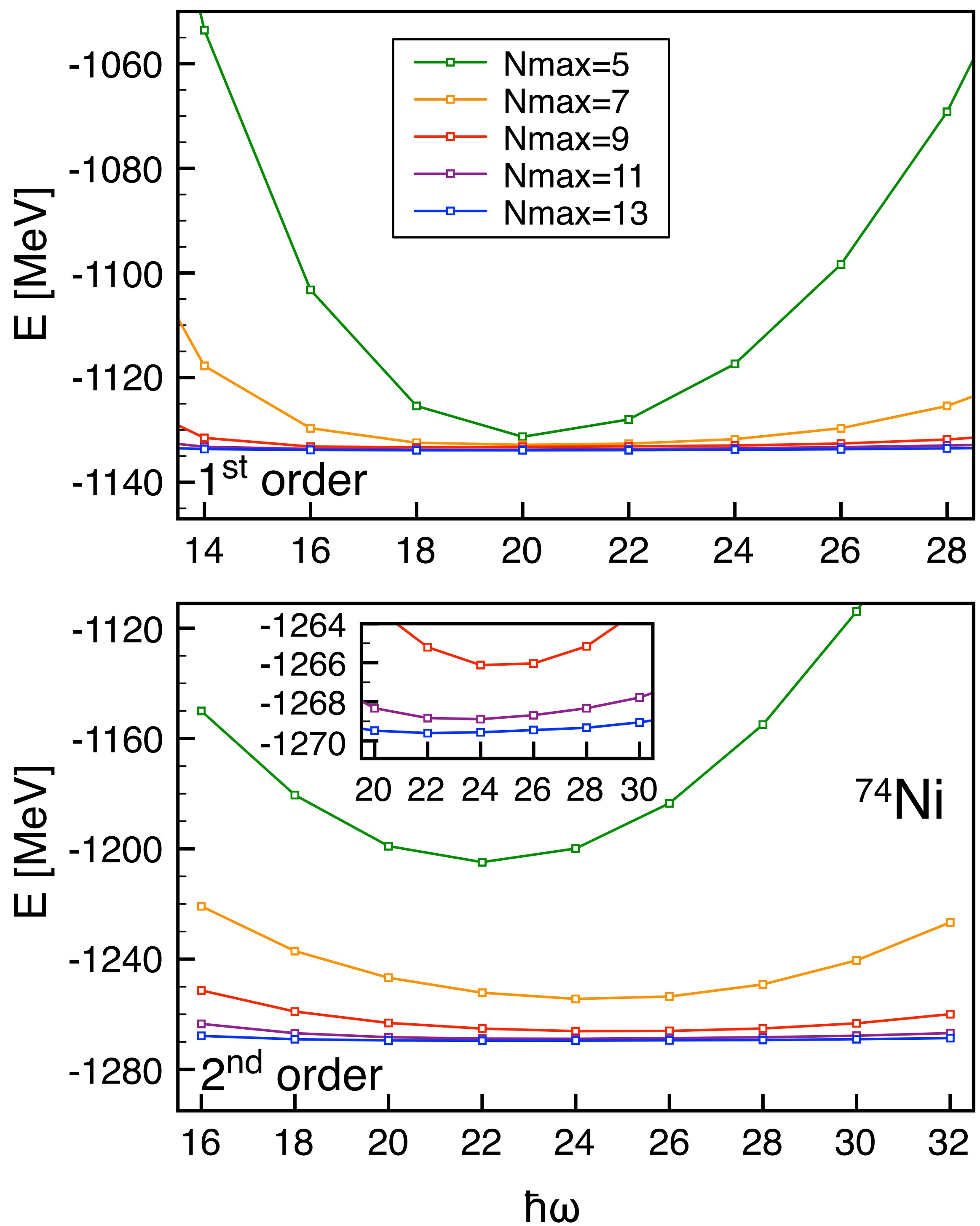


Centroids



Towards medium / heavy open-shell

✳ Case of ^{74}Ni



➟ Very good convergence

➟ From N=13 to N=11 → 200 keV

E (N=13) = -1269.6 MeV
E (N=∞) = -1269.7(2) MeV

(Extrapolation to infinite model space from [Coon *et al.*, 2012; Furnstahl *et al*. 2012])

^{74}Ni - spectral information

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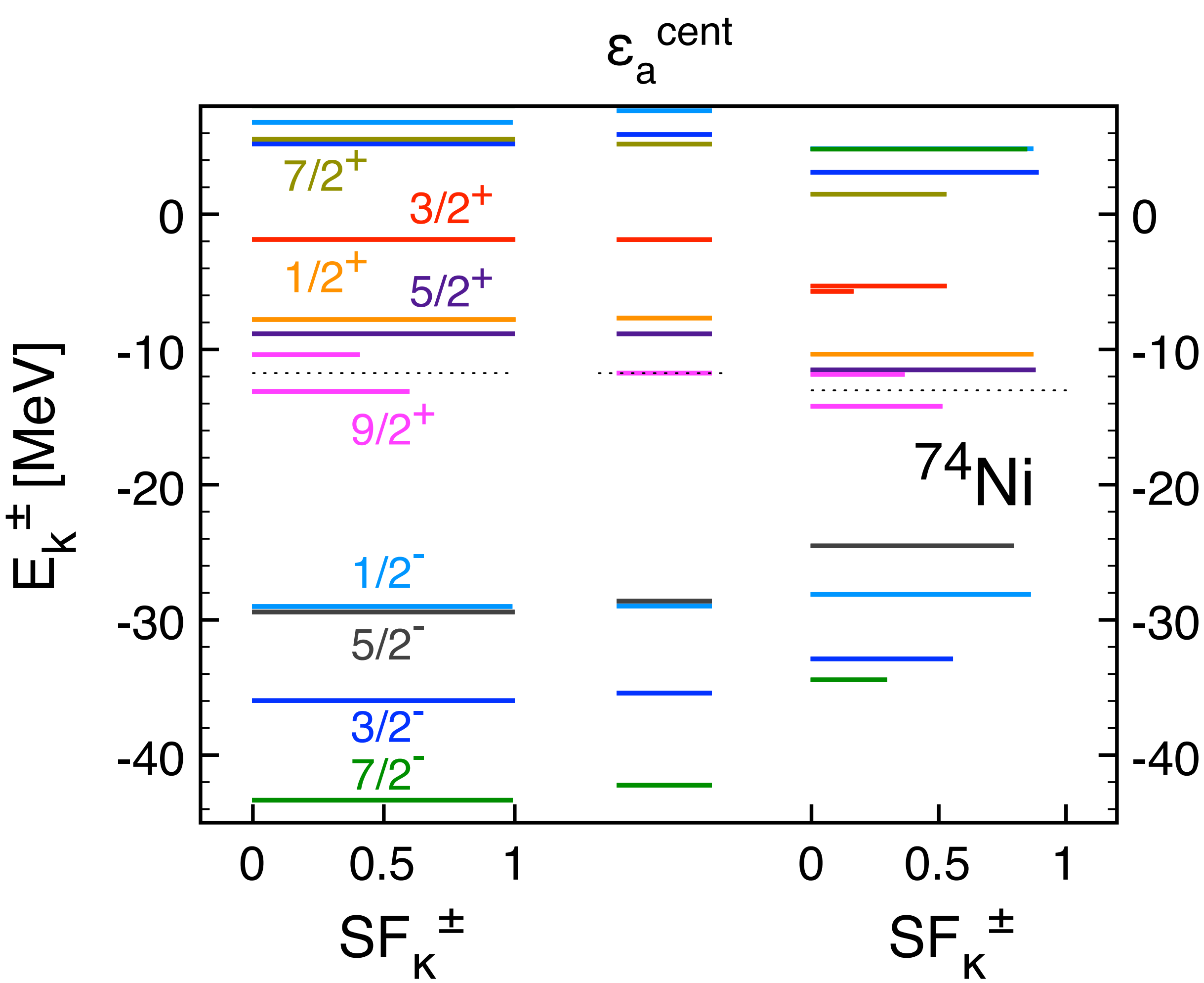
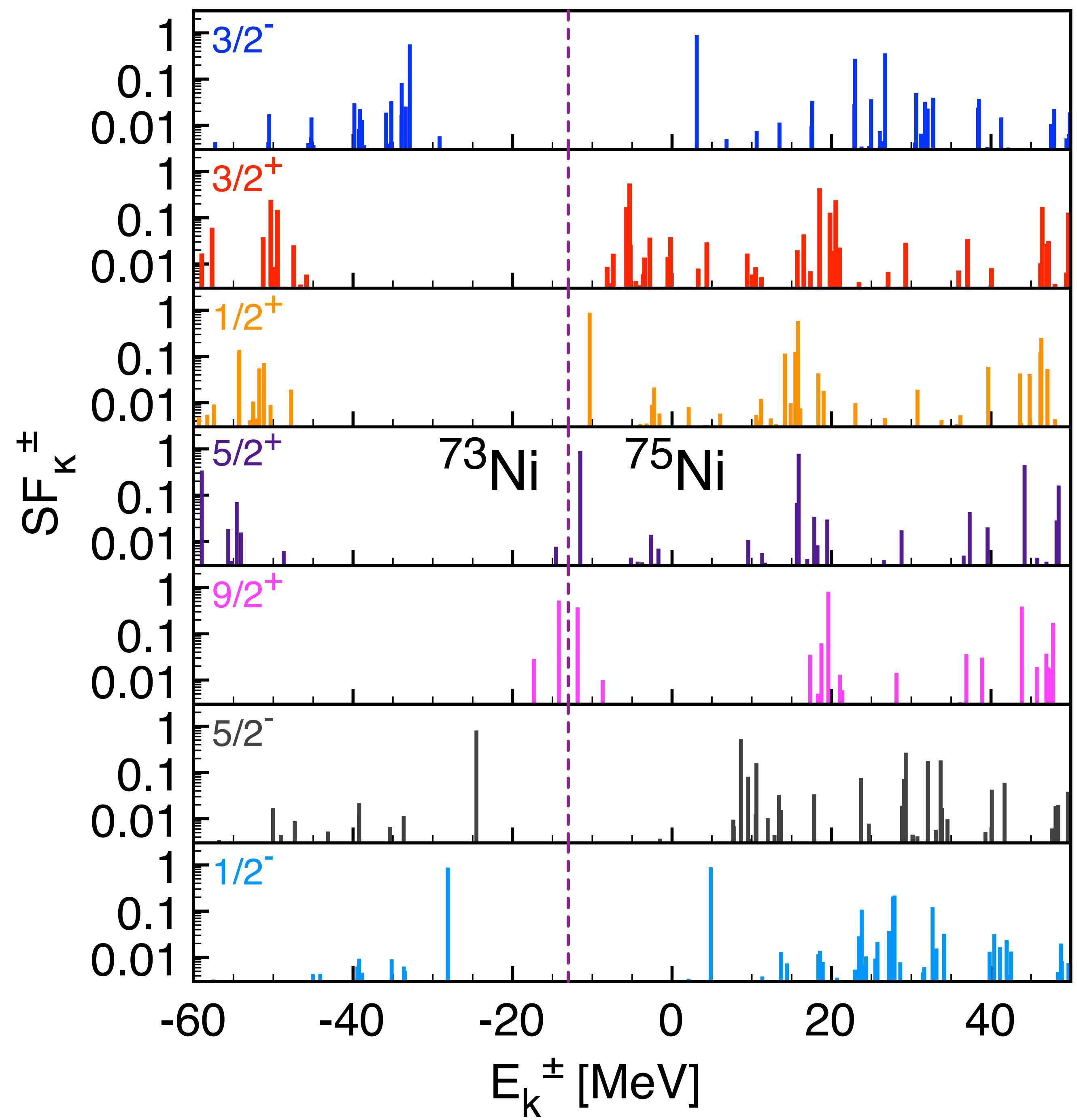
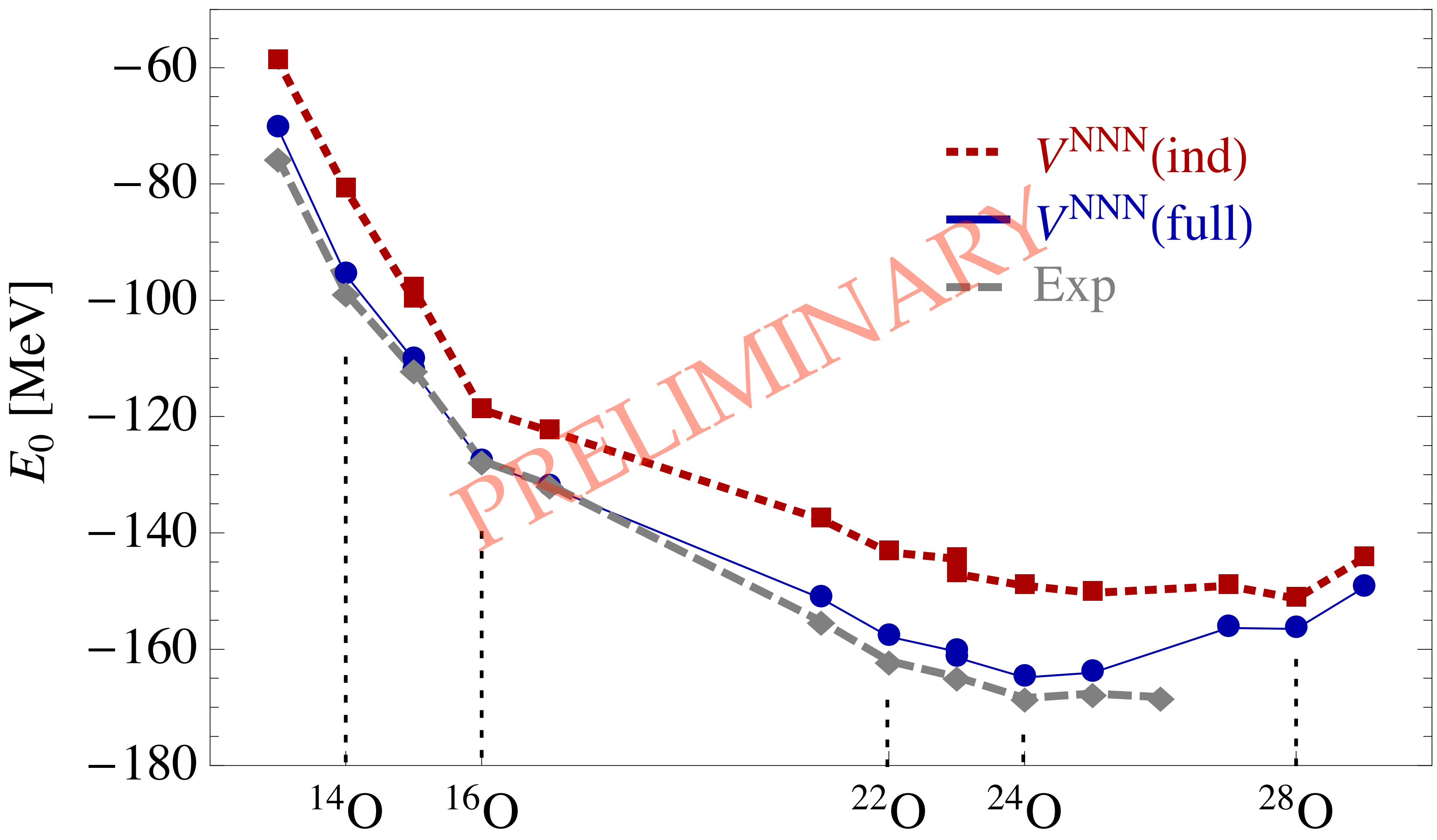
- Static and dynamic pairing correlations
- Second order compresses spectrum
- Many-body correlations screened out from ESPEs





Three-body forces

- 3NF in the Gorkov formalism: work in progress
- Already implemented in Dyson GF



[Cipollone, Barbieri, Navrátil, *in preparation*]

Conclusions and outlook

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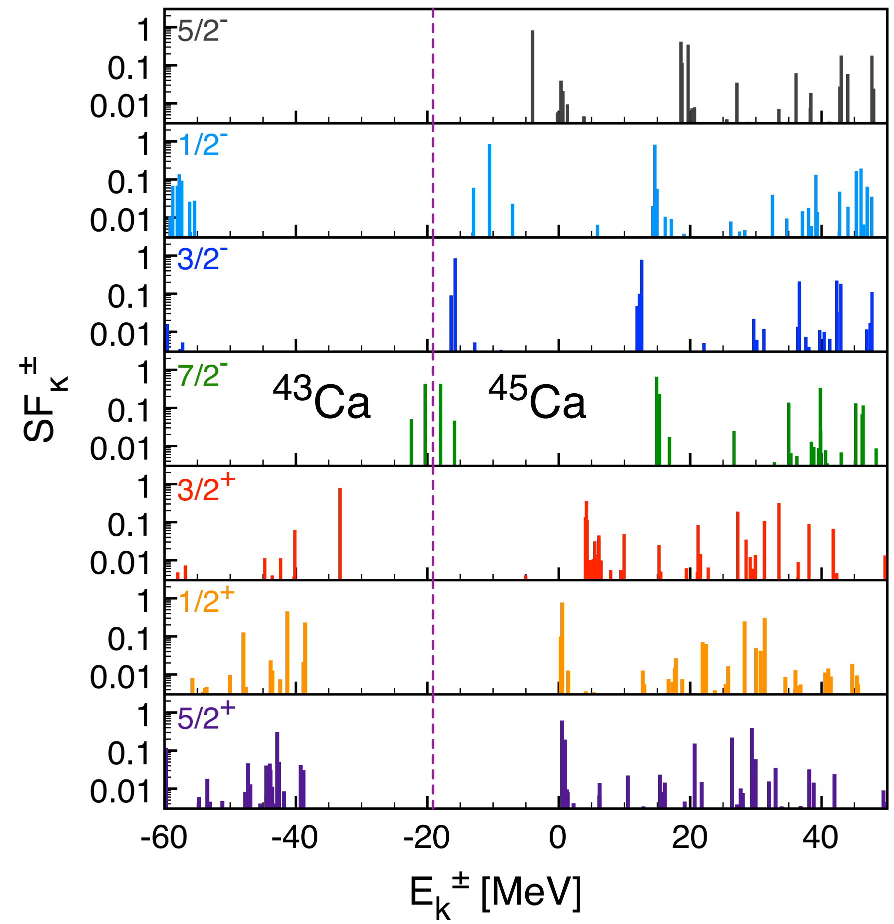
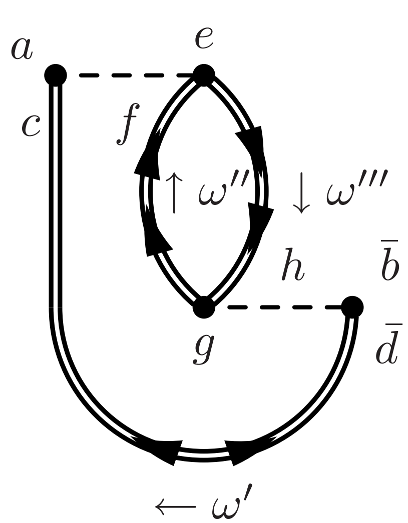
- Gorkov-Green's functions:
  first ab-initio open-shell calculations

- Good convergence, reasonable scaling,
  agreement with CC benchmarks

- Provide a manageable way to address
  (near) degenerate systems





- Implementation of three-body forces

- Proper coupling to the continuum

- Formulation of particle-number restored Gorkov theory

- Improvement of the self-energy expansion