Gorkov-Green's function approach to open-shell systems

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EMMI

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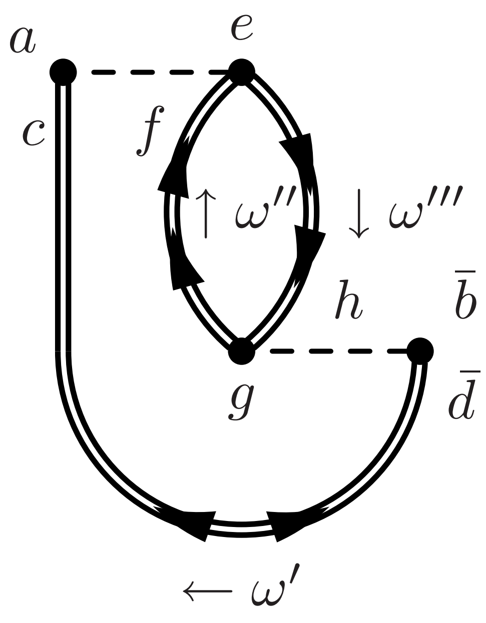
Based on:

- Somà, Duguet, Barbieri, PRC 84 064317 (2011)
- Somà, Barbieri, Duguet, PRC 87 011303(R) (2013)
- Barbieri, Cipollone, Somà, Duguet, Navrátil, arXiv:1211.3315
- Somà, Barbieri, Duguet, arXiv:1304.xxxx
- Somà, Cipollone, Barbieri, Duguet, Navrátil, *in preparation*



INT Workshop

Advances in many-body theory: from nuclei to molecules

Seattle, 4 April 2013

Towards a first-principle description of nuclei

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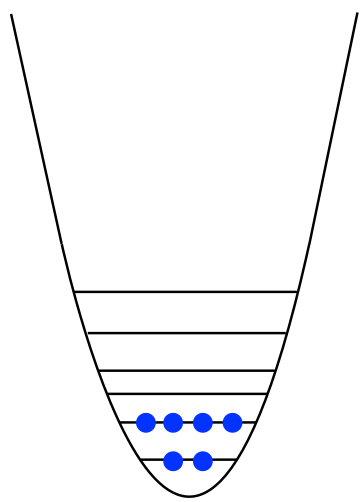
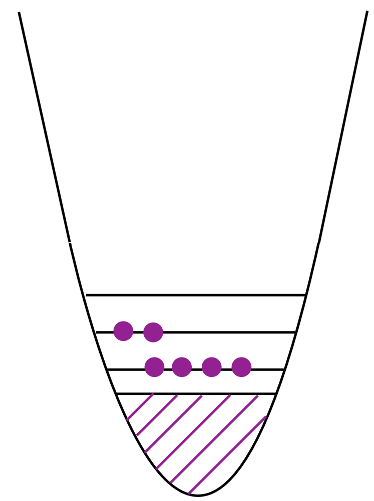
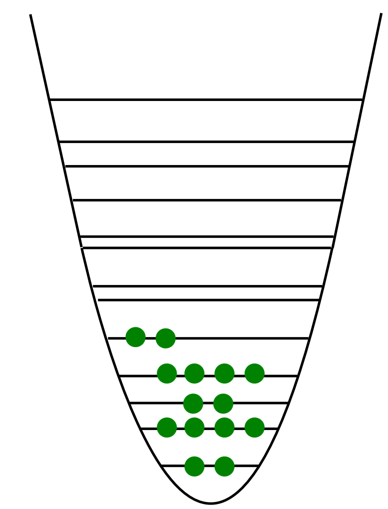
Light nuclei	Medium-mass nuclei	Medium-mass nuclei
		
NCSM, GFMC, ...	Miscroscopic SM, ...	GF, CC, IM-SRG, ...

Configuration interaction limited to small valence/model spaces

Usual expansion schemes fail to account for pairing correlations

Limited to to doubly-closed-shell ± 1 and ± 2 nuclei

Error estimates in *ab initio* calculations

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- Long-term goal: predictive nuclear structure calculations
  - ➠ With quantified theoretical errors
  - ➠ Consistent description of structure and reaction

- Estimation of theoretical errors in *ab initio* methods

	Gorkov GF
1) Hamiltonian	✘
2) Many-body expansion	✘
3) Model space truncation	✔
4) Numerical algorithms	✔

Paths to open-shell systems

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✪ Two ways to address (near)-degenerate systems

(a) Multi-reference approaches

➟ e.g. IMSRG + CI, MR-CC, microscopic VS-SM

(b) Single-reference approaches

➟ explicit account of pairing mandatory

Self-consistent Gorkov-Green's functions:

✪ Bogoliubov algebra + Green's function theory

✪ Address explicitly the non-perturbative physics of Cooper pairs

➟ Formulate the expansion scheme around a Bogoliubov vacuum

➟ Breaking of particle-number conservation (eventually restored)

Gorkov's framework

✪ 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 $\Omega = H - \mu A$

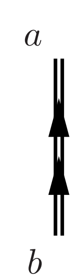
➟ $|\Psi_0\rangle$ minimizes $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$ under the constraint $A = \langle \Psi_0 | A | \Psi_0 \rangle$

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

✪ Set of 4 Green's functions

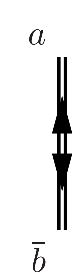
[Gorkov 1958]

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

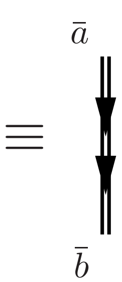


$$i \, G^{21}_{ab}(t,t') \equiv \langle \Psi_0 | T \left\{ \bar{a}_a^\dagger(t) a_b^\dagger(t') \right\} | \Psi_0 \rangle \quad \equiv$$

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



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



Spectrum and spectroscopic factors

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✪ 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

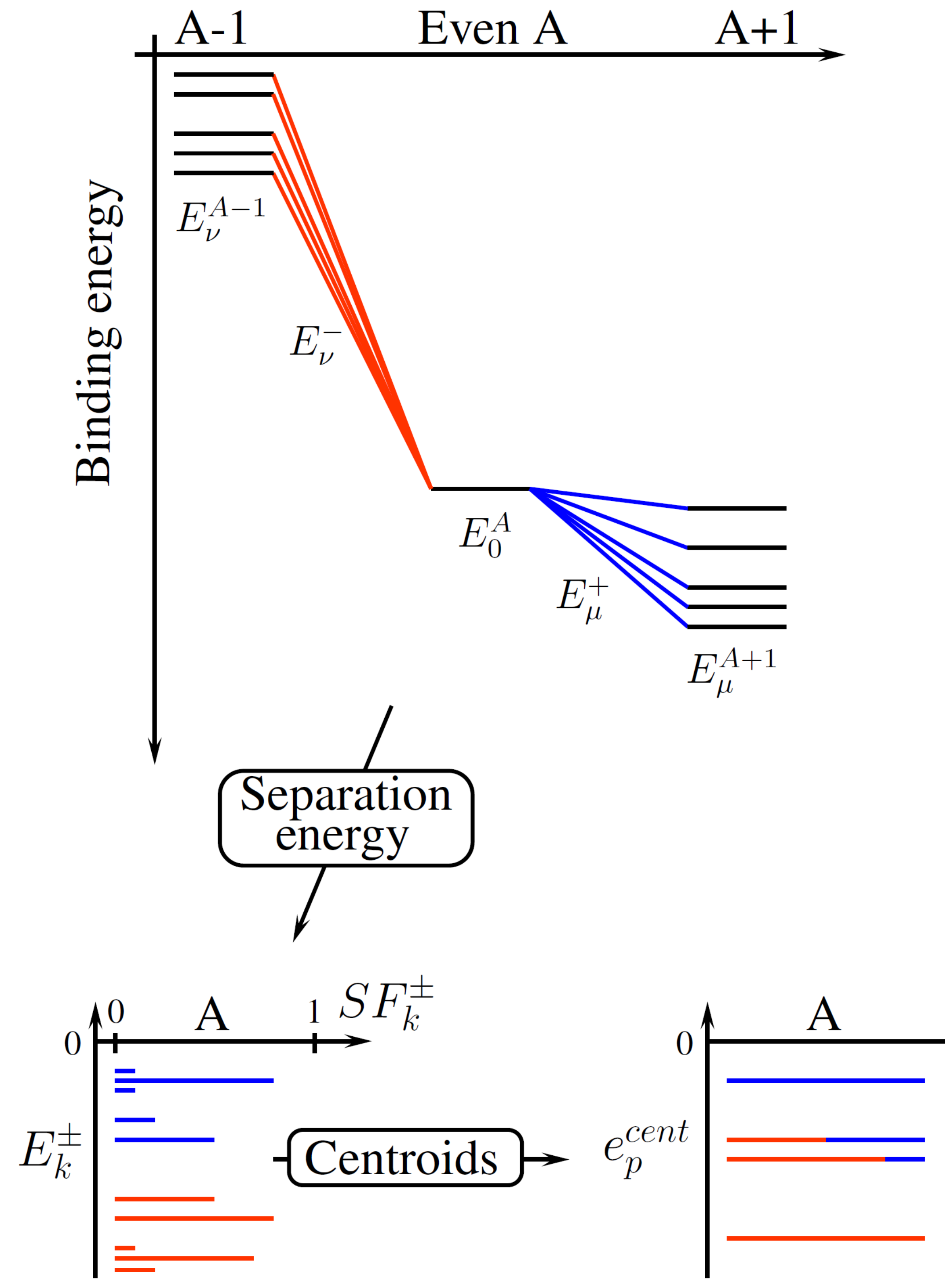
where
$$\begin{cases} \mathcal{U}^{k*}_a \equiv \langle \Psi_k | a^\dagger_a | \Psi_0 \rangle \\ \mathcal{V}^{k*}_a \equiv \langle \Psi_k | \bar{a}_a | \Psi_0 \rangle \end{cases}$$

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]

Self-energy expansion

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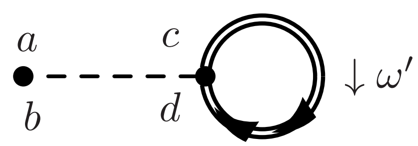
✪ Gorkov equations ⟶ energy *dependent* eigenvalue problem

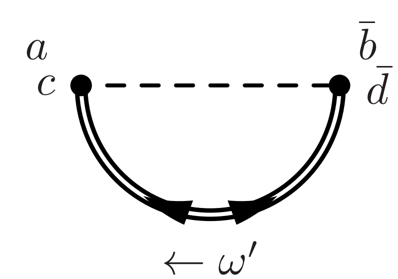
$$\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & -t_{ab} + \mu_{ab} + \Sigma^{22}_{ab}(\omega) \end{pmatrix}\Bigg|_{\omega_k} \begin{pmatrix} \mathcal{U}^k_b \\ \mathcal{V}^k_b \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k_a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

✪ 1st order ➟ energy-independent self-energy

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

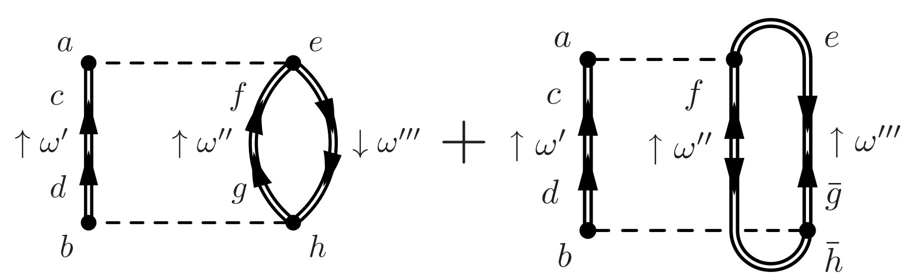


$\Sigma^{12\,(1)}_{ab} =$

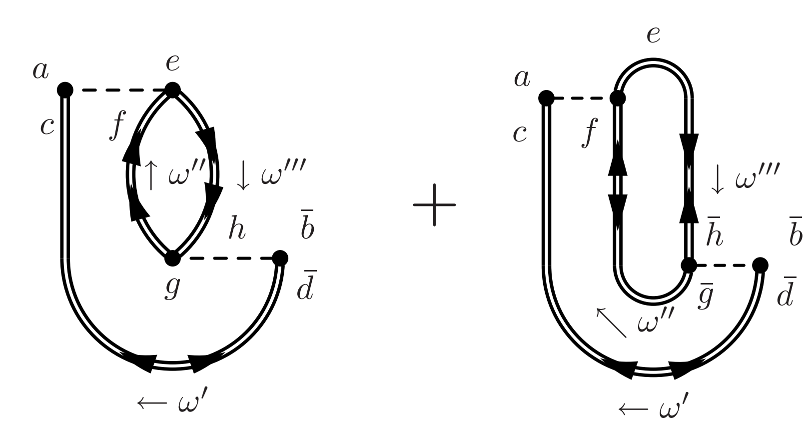


✪ 2nd order ➟ energy-dependent self-energy

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



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



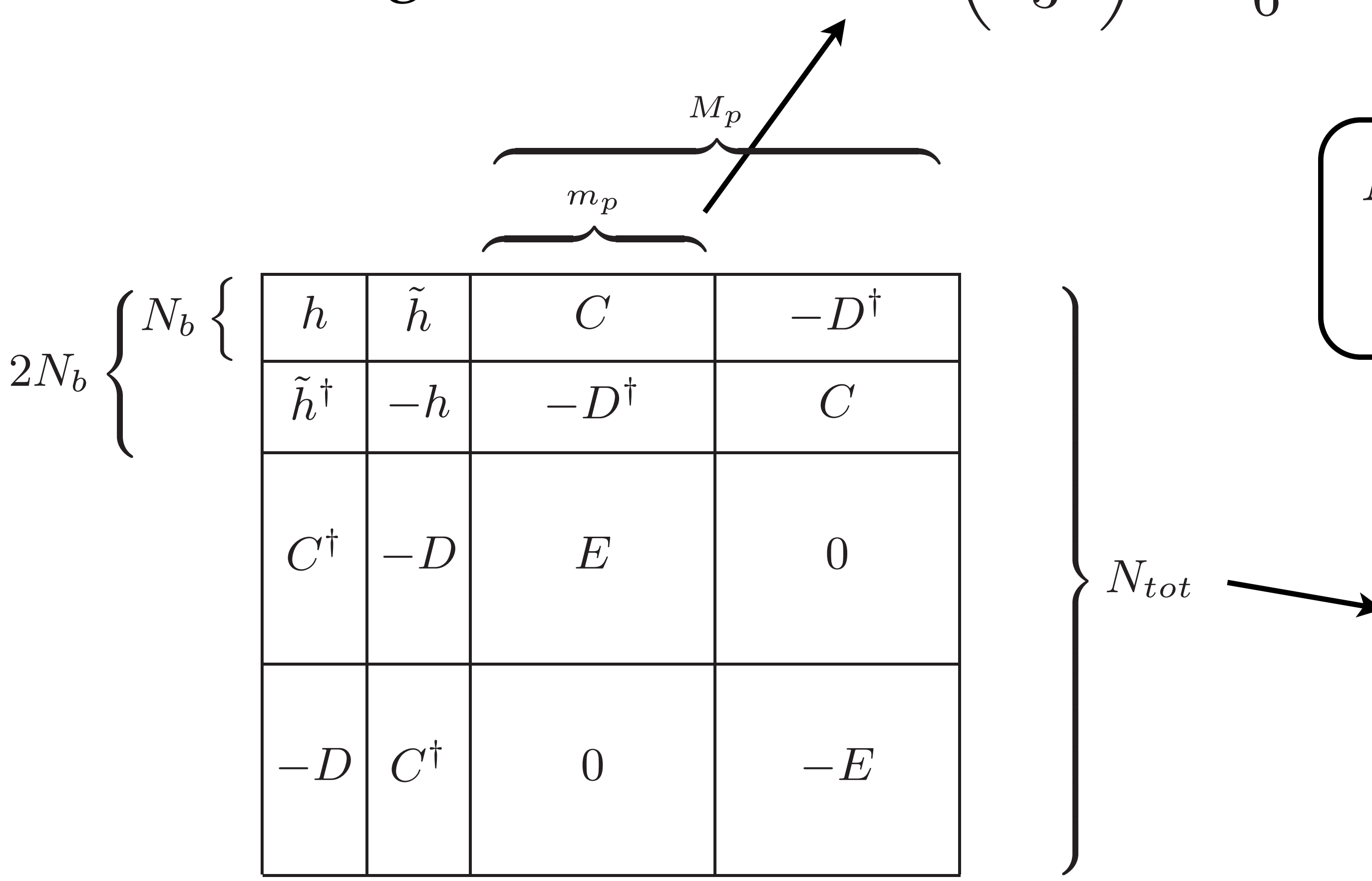
Scaling of Gorkov's problem

✪ 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

$$m_{p,1} \approx \begin{pmatrix} N_b \\ 3 \end{pmatrix} \propto \frac{N_b^3}{6}$$



N_b → dimension of the s.p. basis

n → number of iterations

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

$$\ldots$$

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

Tame the dimension growth

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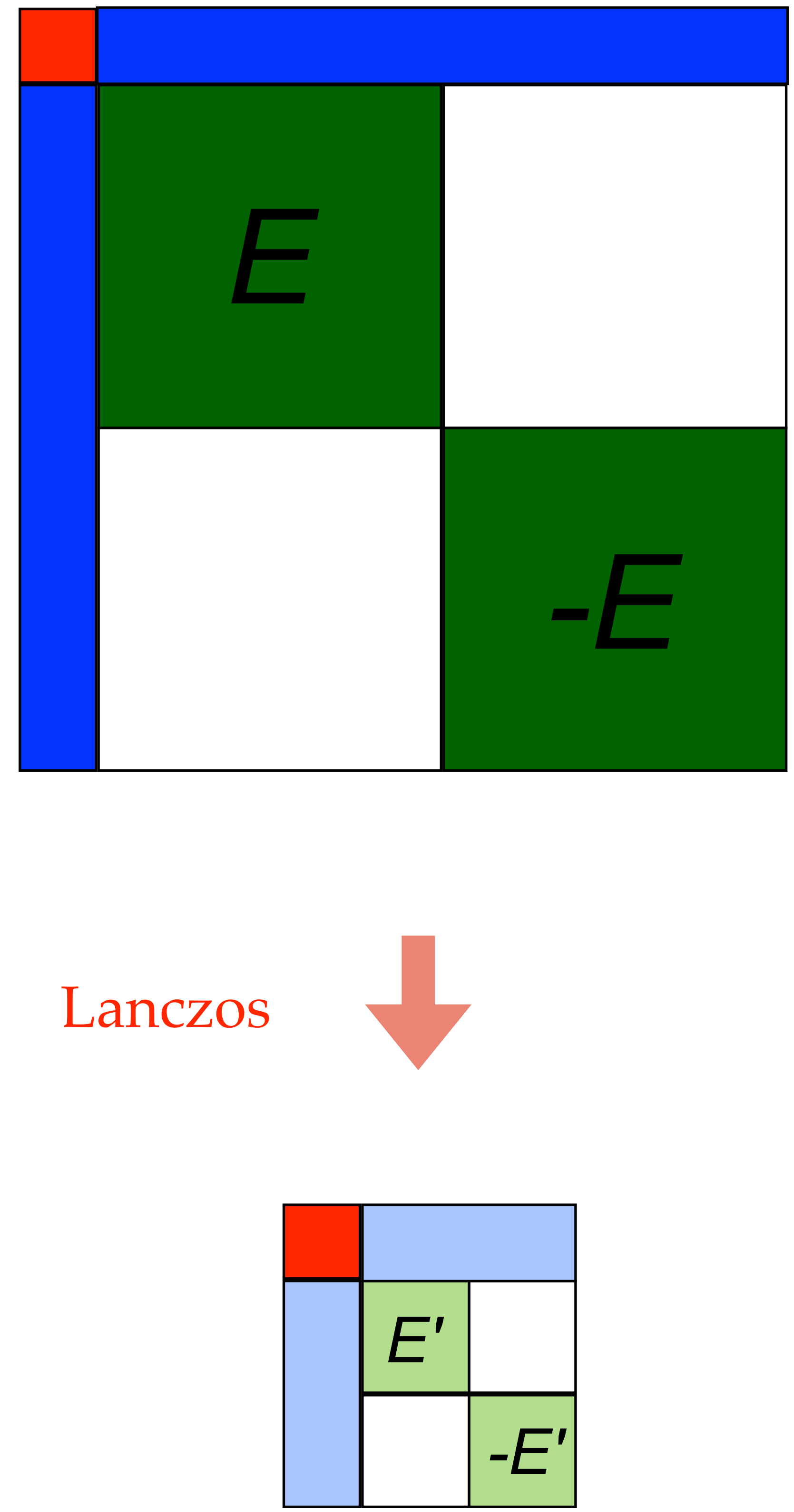
✪ How do we select the poles?

We do not...

Krylov 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 $N_l \rightarrow \dim(E)$

Testing Krylov projection

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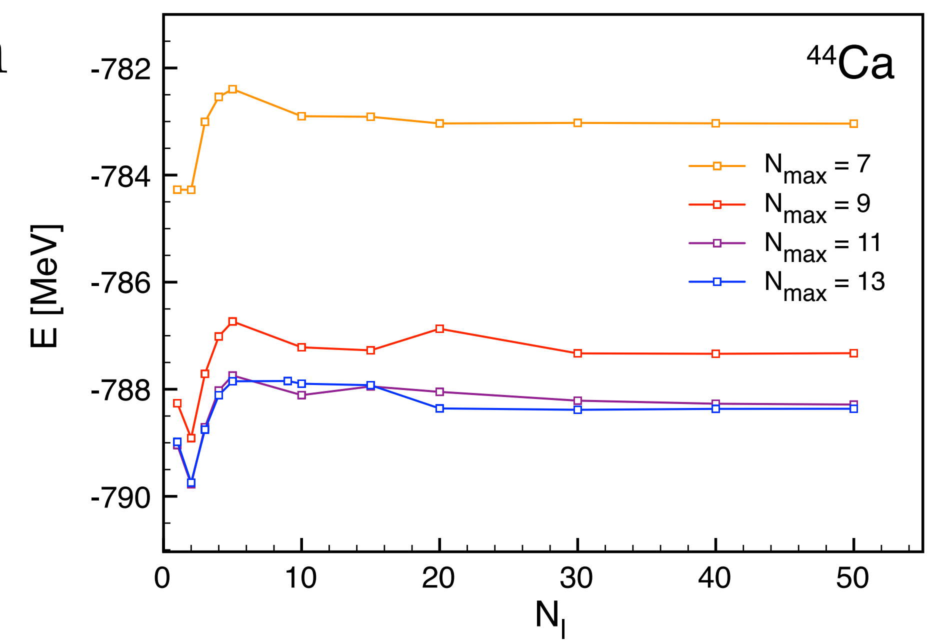
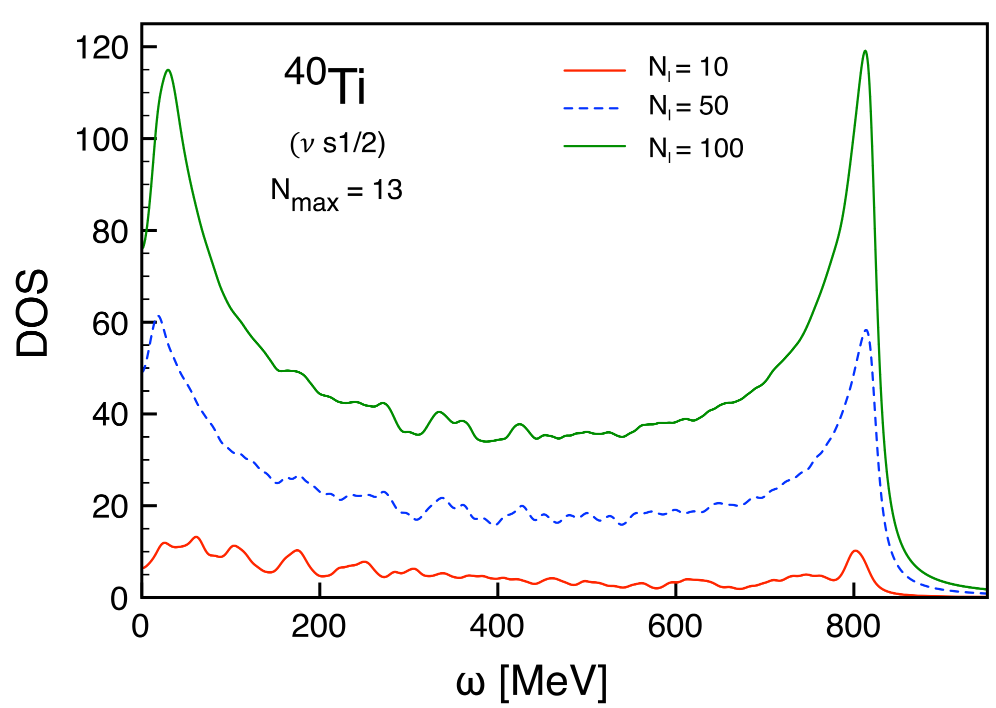
- Energy and spectral independent of the projection
- Same behavior for all model spaces

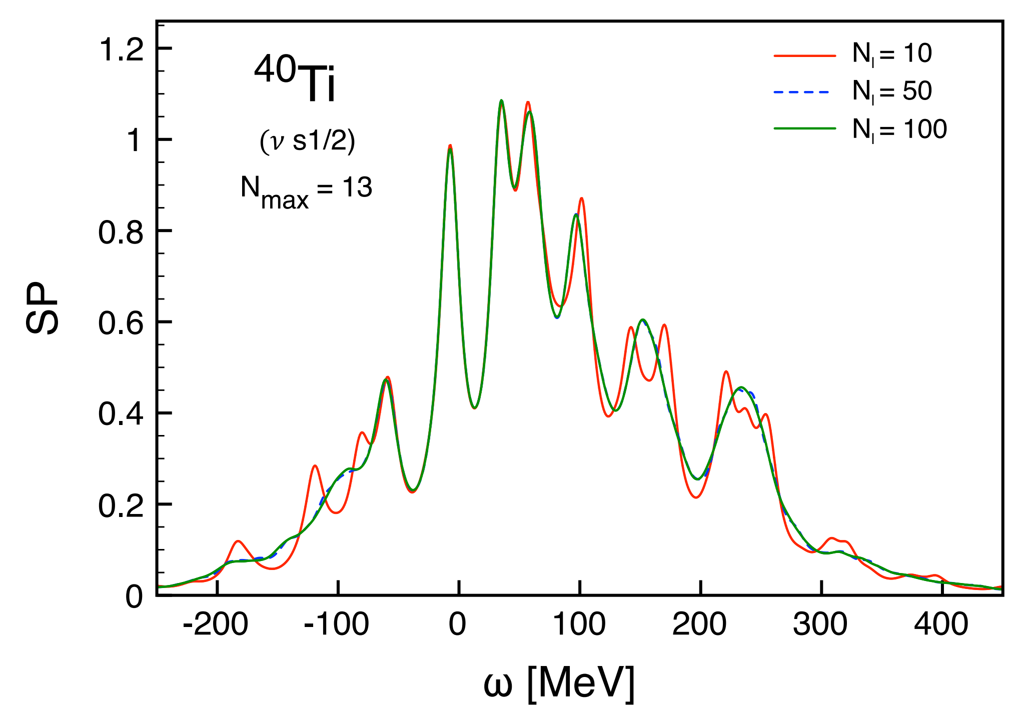
favorable scaling



Density of states

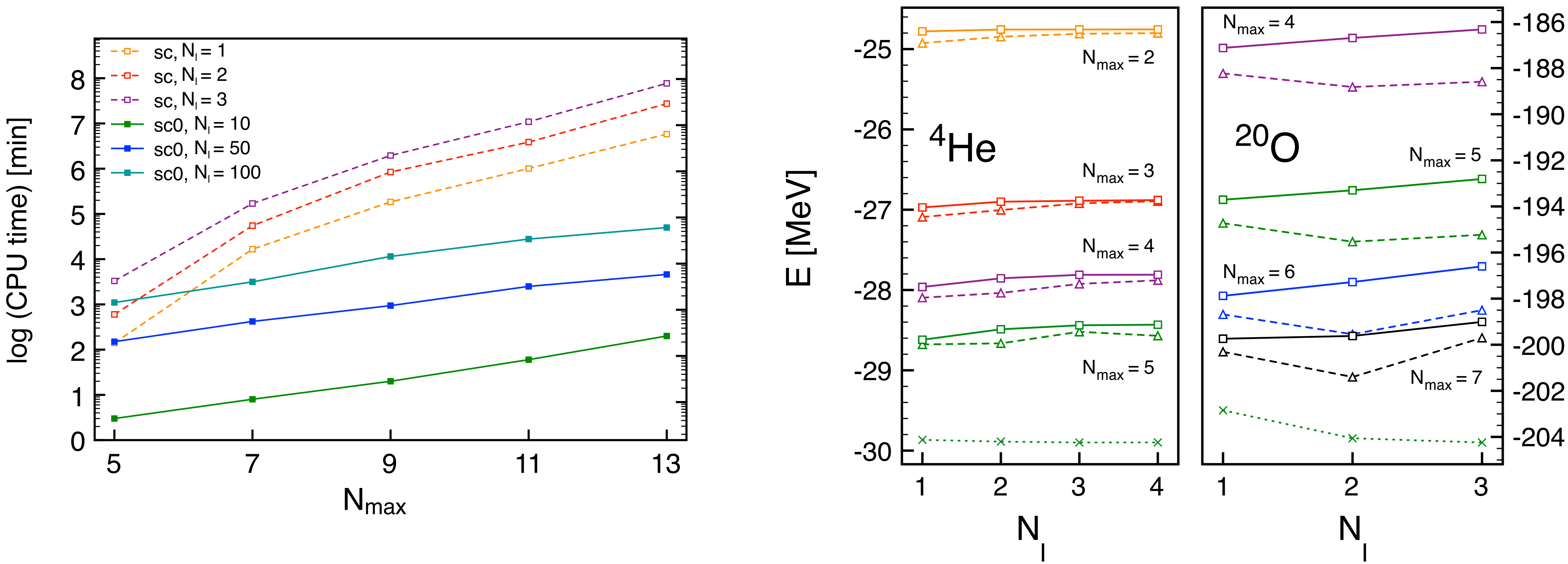


Spectral strength



Self-consistency and scaling

✪ Fully (dashed) vs. partially (solid) SC



➟ Scaling does not depend on A

➟ Partial self-consistency grasps most of the correlations

➟ MBPT(2) inadeguate

Towards medium / heavy open-shell

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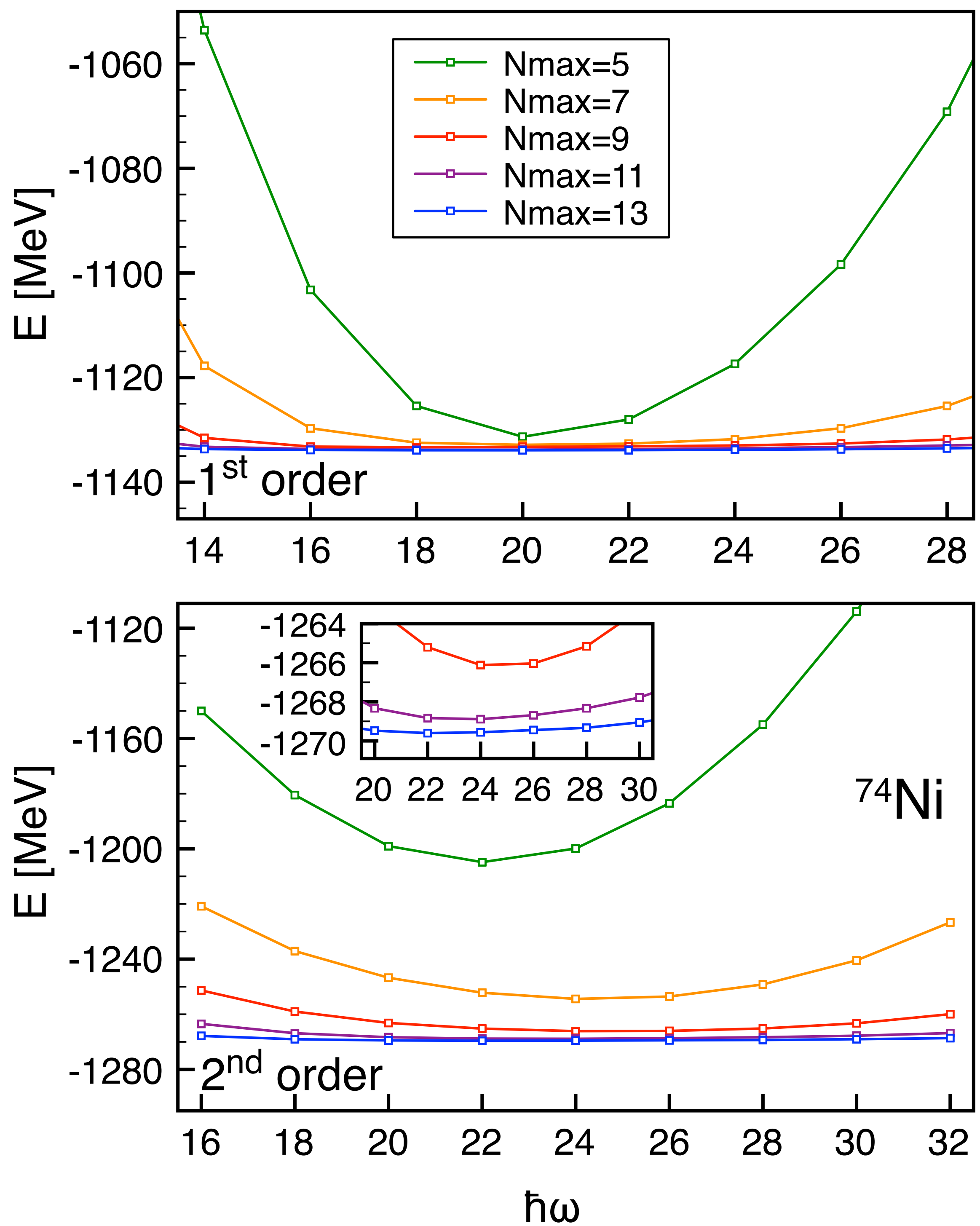
✪ ^{74}Ni



➟ NN interaction:
chiral N^{3}LO SRG-evolved to 2.0 fm^{-1}

[Entem and Machleidt 2003]

➟ Very good convergence

➟ From N=13 to N=11 → 200 keV

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

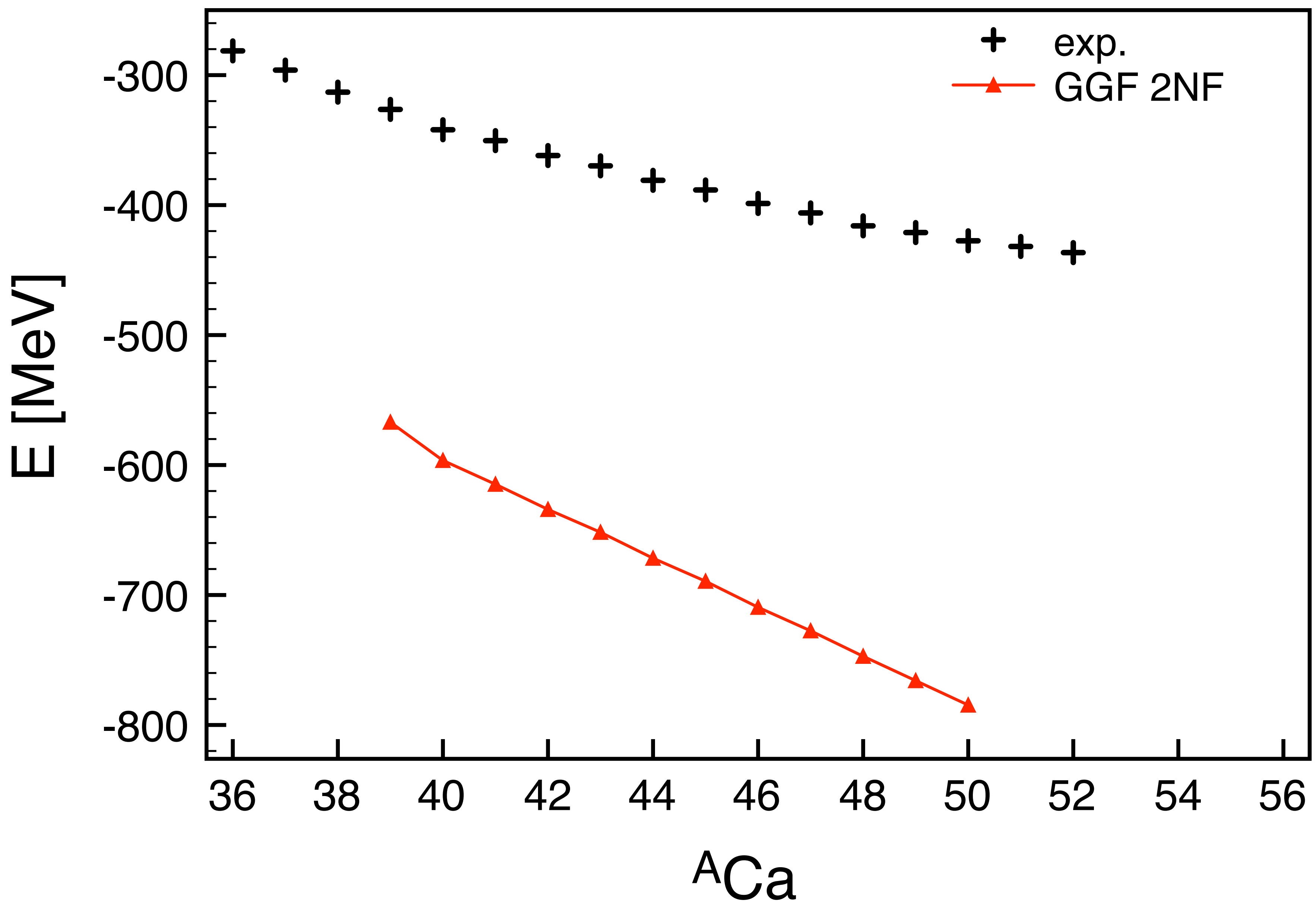
(Extrapolation to infinite model space from [Furnstahl, Hagen, Papenbrok 2012] and [Coon et al. 2012])

Calcium isotopic chain

✪ NN only

➟ Systematic along isotopic/isotonic becomes available

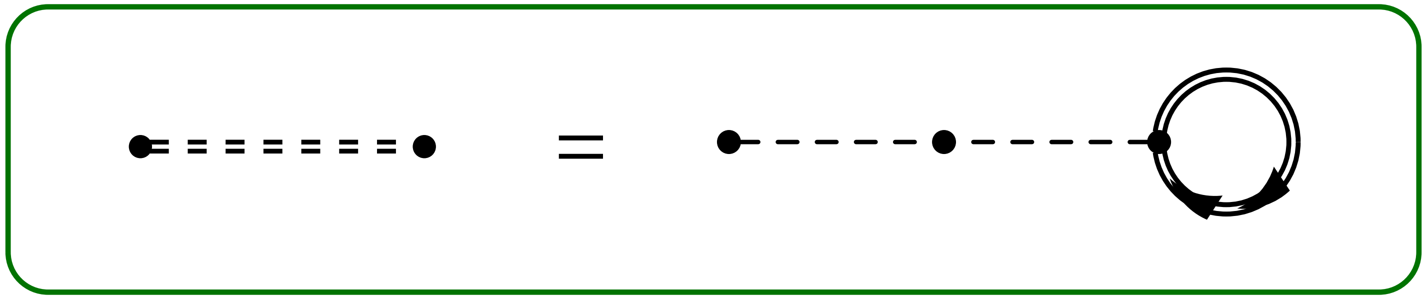
➟ Overbinding (increasing with A): need for three-body forces



Three-body forces

✪ Inclusion of 3NF as effective 2NF

➟ Average over the 3rd nucleon in each nucleus



➟ Additional term in the Galitskii-Koltun sum rule [Cipollone *et al*. 2013]

$$E_0^{\mathrm{A}} = \frac{1}{4\pi i}\int_{C\uparrow} d\omega\, \mathrm{Tr}_{\mathcal{H}_1}\left[\mathbf{G}^{11}(\omega)\,[\mathbf{T}+(\mu+\omega)\;\mathbf{1}]\right] - \frac{1}{2}\langle\Psi_0|W|\Psi_0\rangle$$

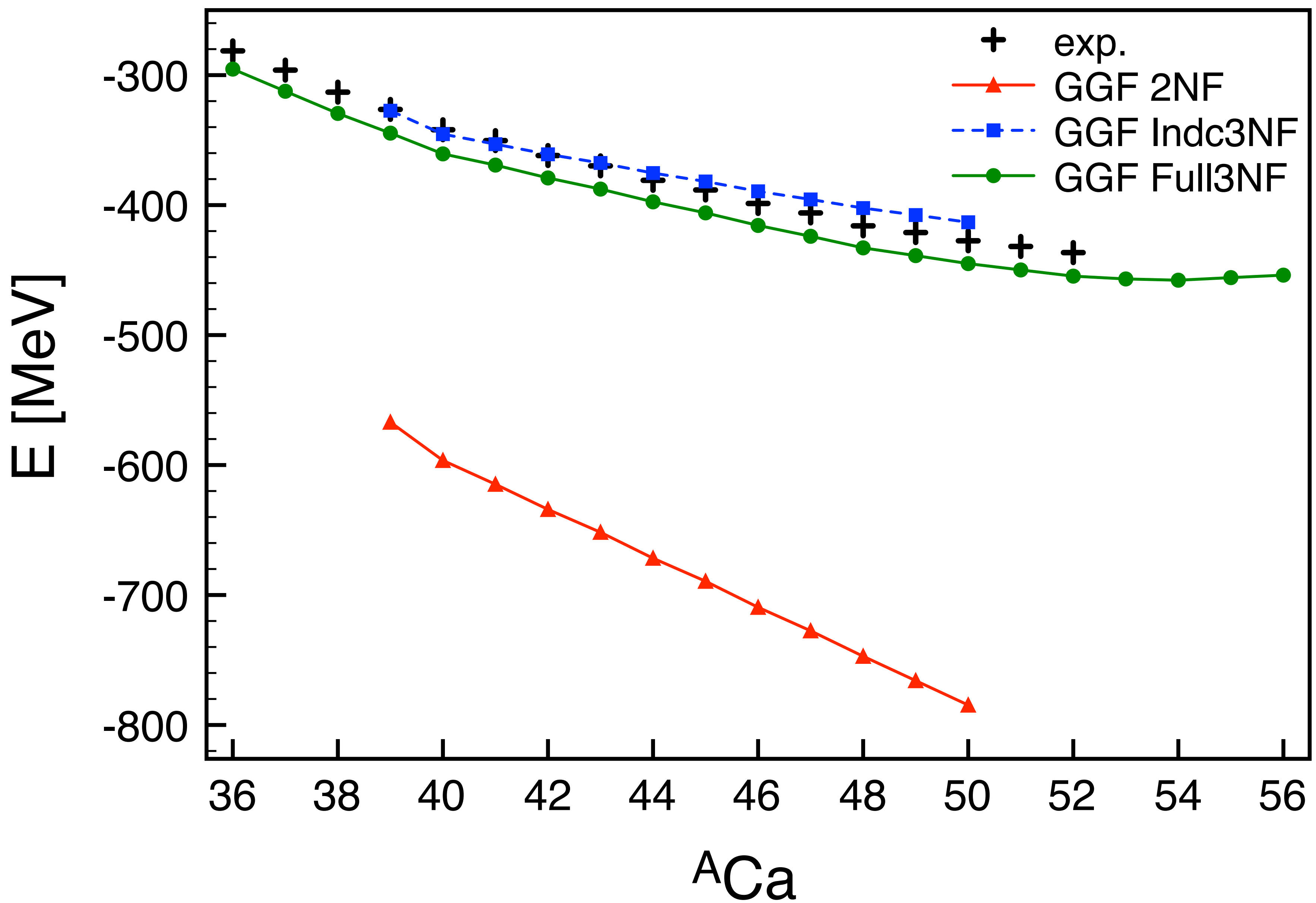
✪ 3N interaction: chiral N^{2}LO (400 MeV) SRG-evolved to 2.0 fm^{-1} [Navrátil 2007]

➟ Fit to three- and four-body systems only

➟ Modified cutoff to reduce induced 4N contributions [Roth *et al*. 2012]

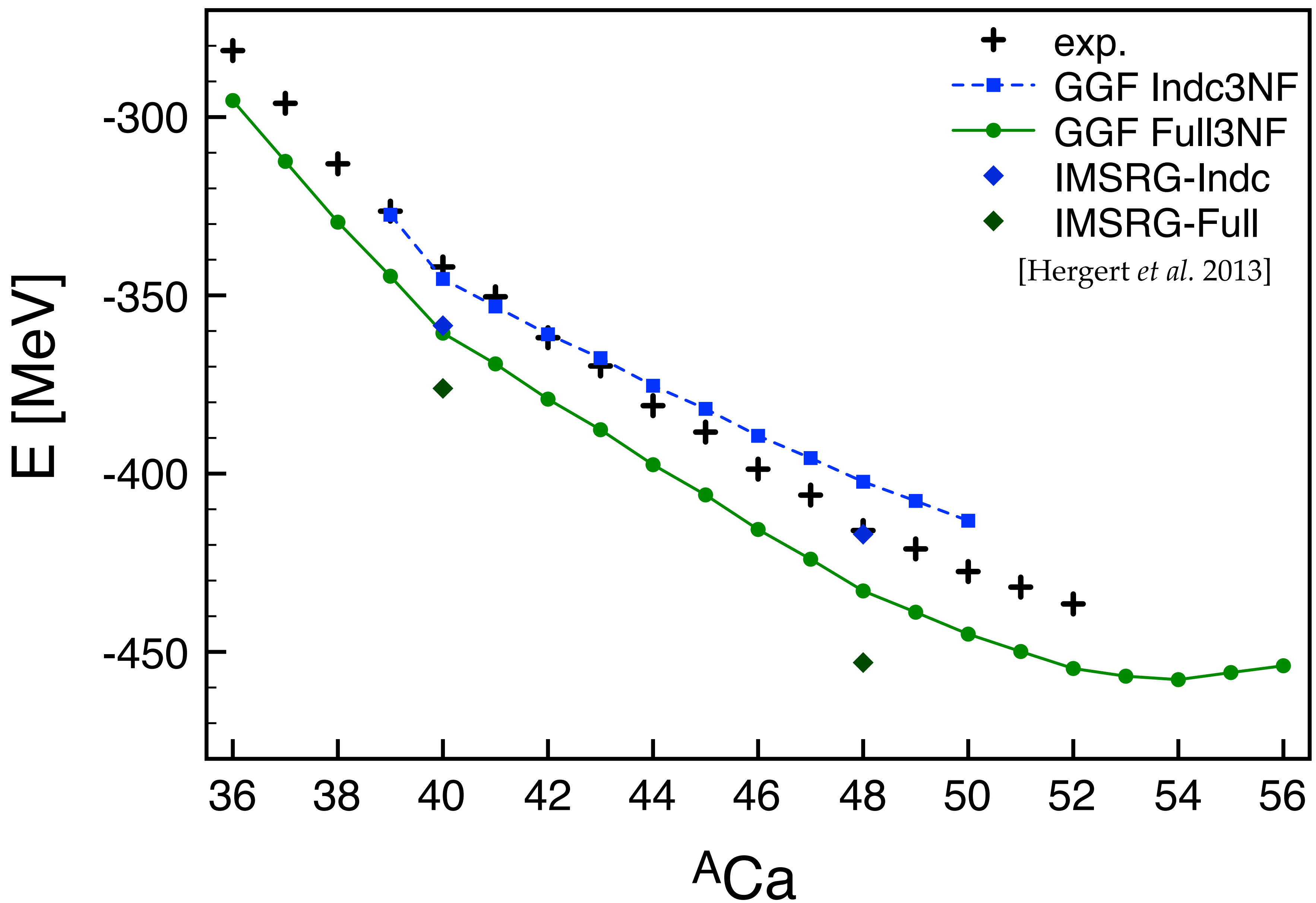
Calcium isotopic chain

- ✪ First *ab initio* calculation of the whole Ca chain with NN + 3N forces
  - ➟ 3NF bring energies close to experiment
  - ➟ Induced 3NF and full 3NF investigated



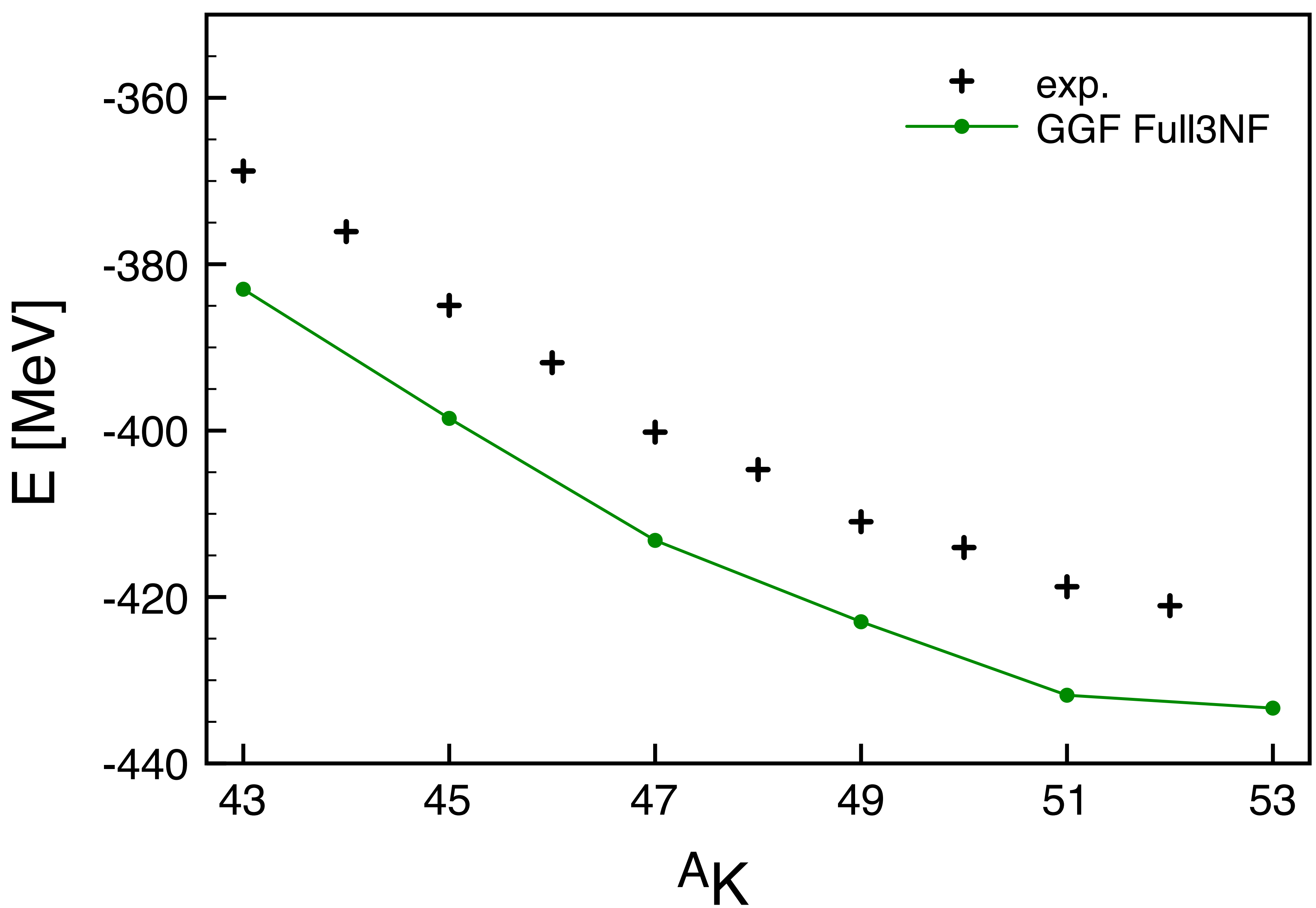
Calcium isotopic chain

- Original 3NF correct the energy curvature
- Good agreement with IM-SRG (quantitative when 3rd order included)



Potassium isotopic chain

- Exploit the odd-even formalism: application to K
  - ➟ Trend and agreement similar to calcium
  - ➟ Future: consistent description of medium-mass driplines

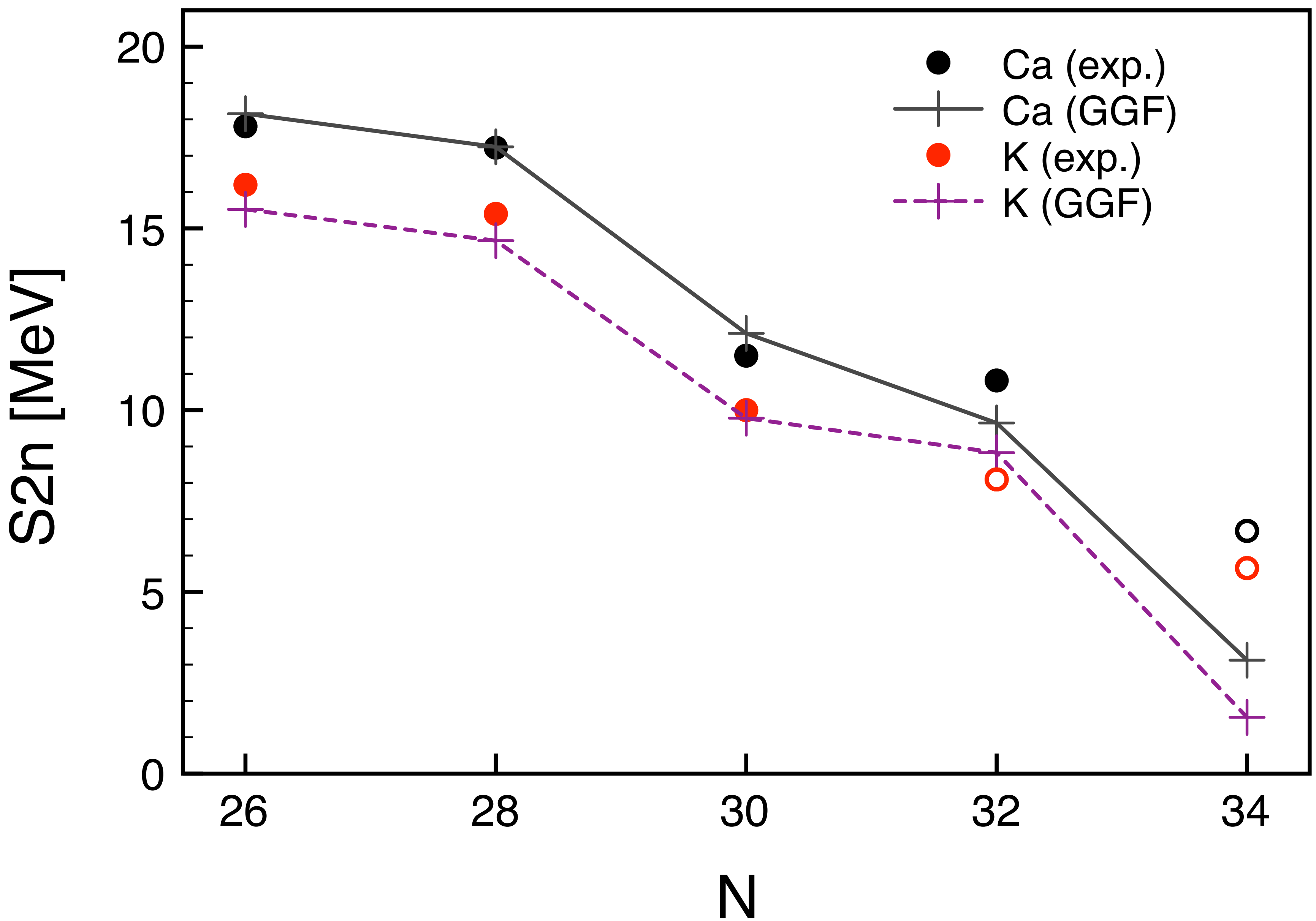


Two-neutron separation energies

✪ Neutron-rich extremes of the nuclear chart

➟ Good agreement with measured S2n

➟ Towards a quantitative *ab initio* description of the medium-mass region



Pairing gaps

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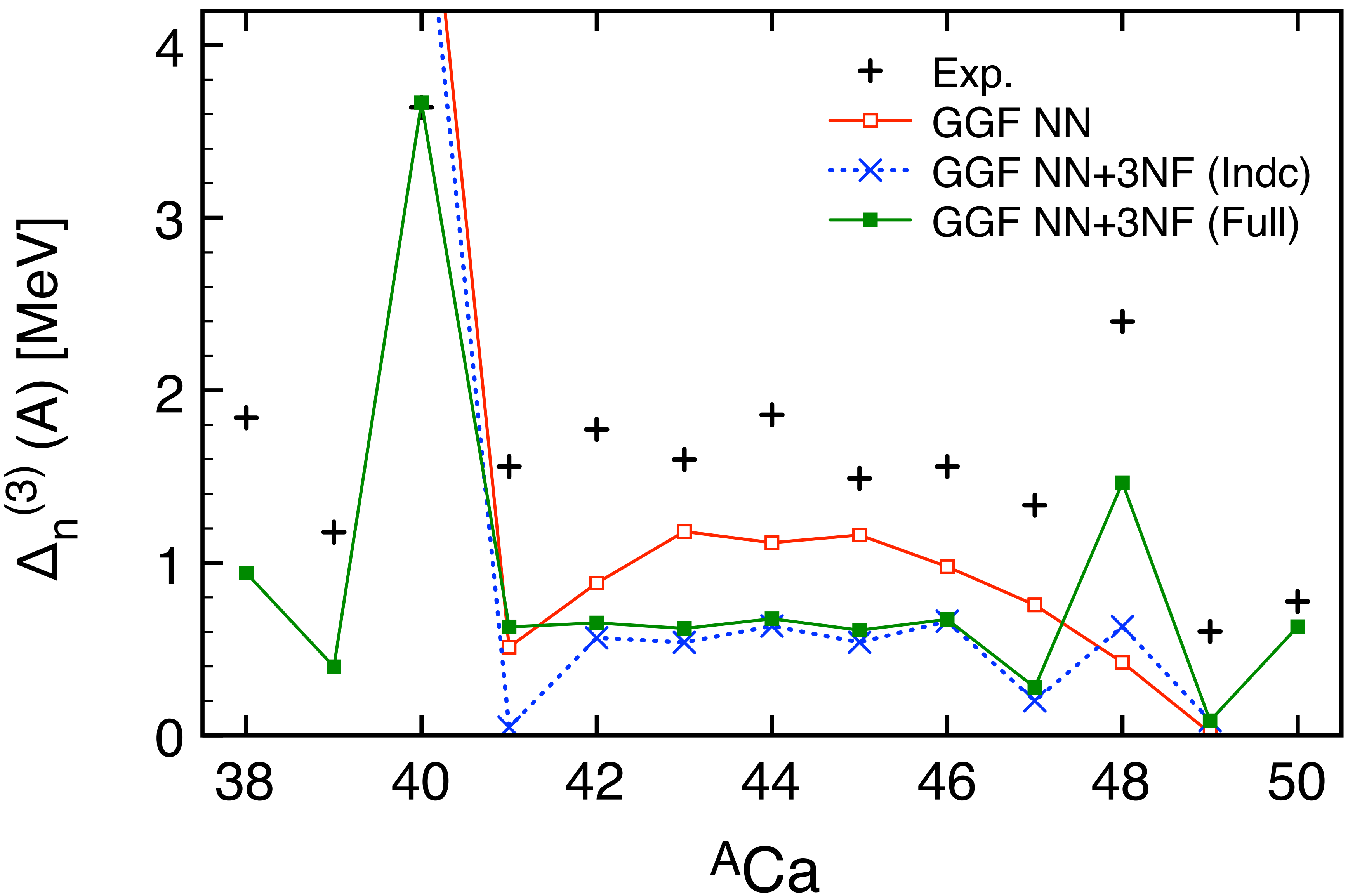
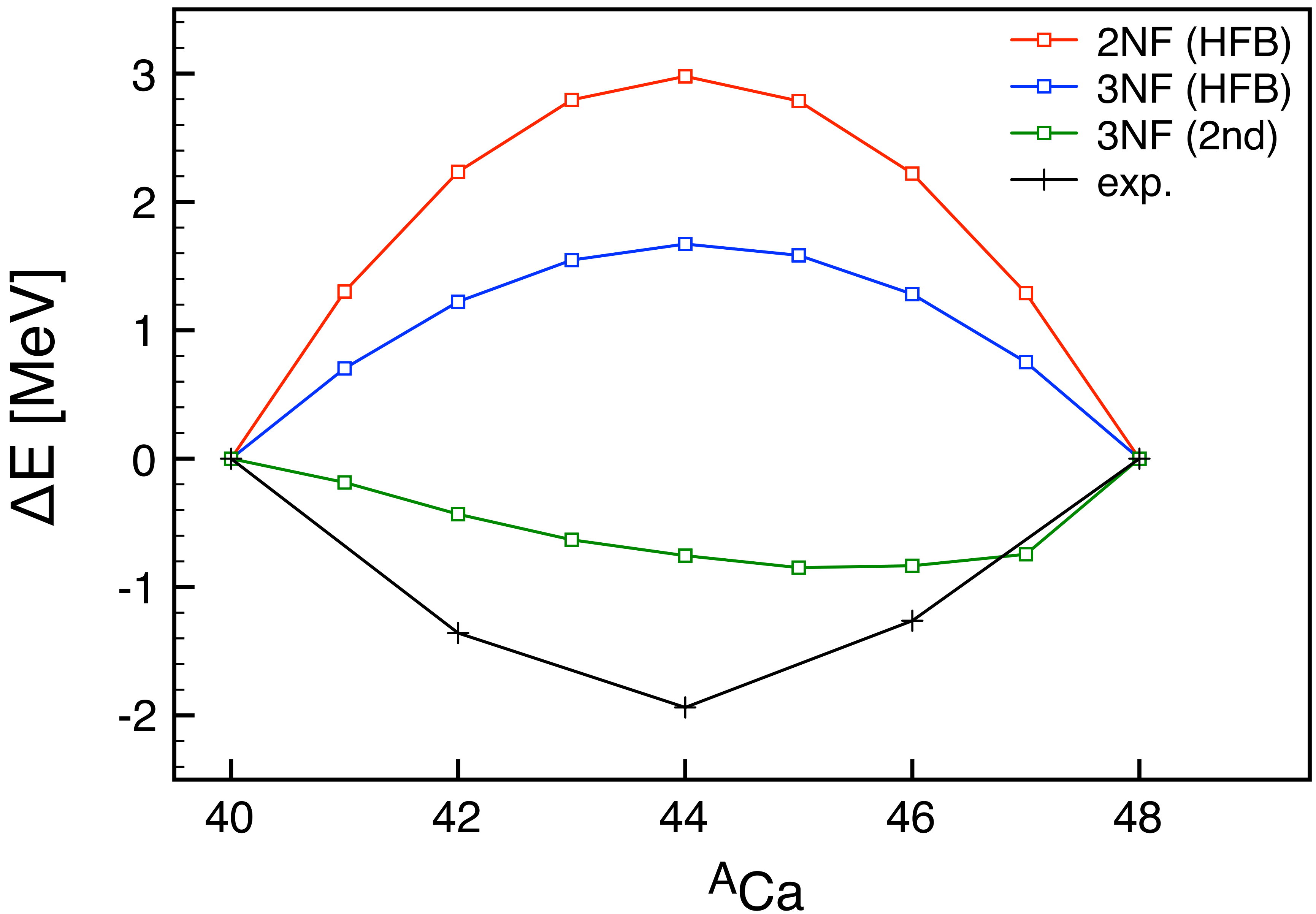
✪ Three-point mass differences

$$\Delta_n^{(3)}(A) = \frac{(-1)^A}{2}[E_0^{A+1} - 2\,E_0^A + E_0^{A-1}]$$



Pairing gaps

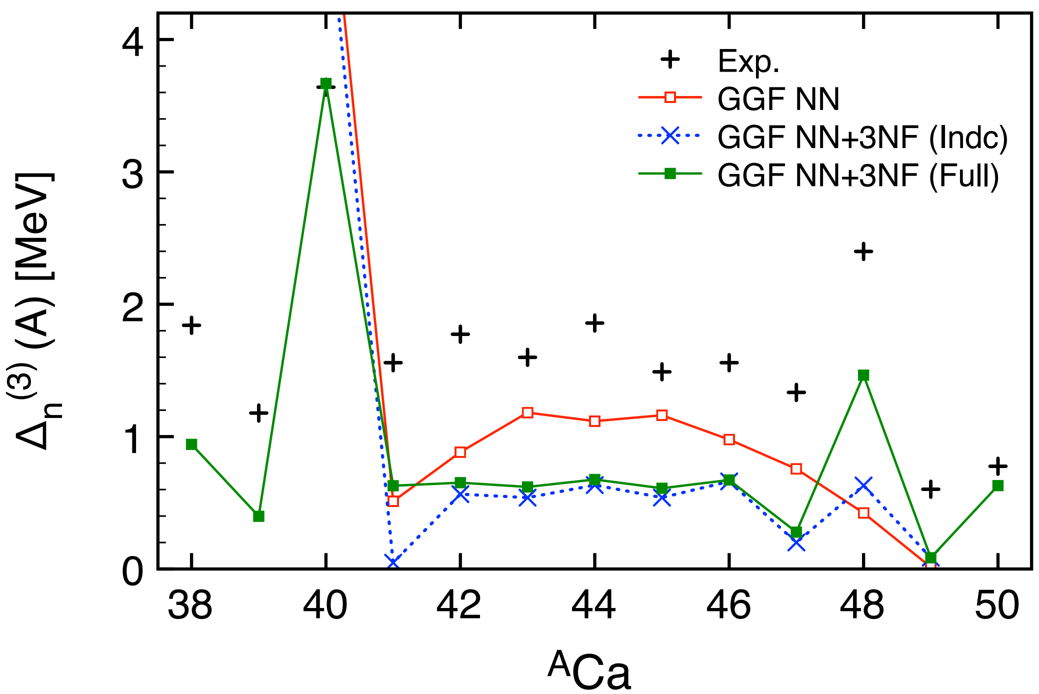
✪ Inversion of odd-even staggering

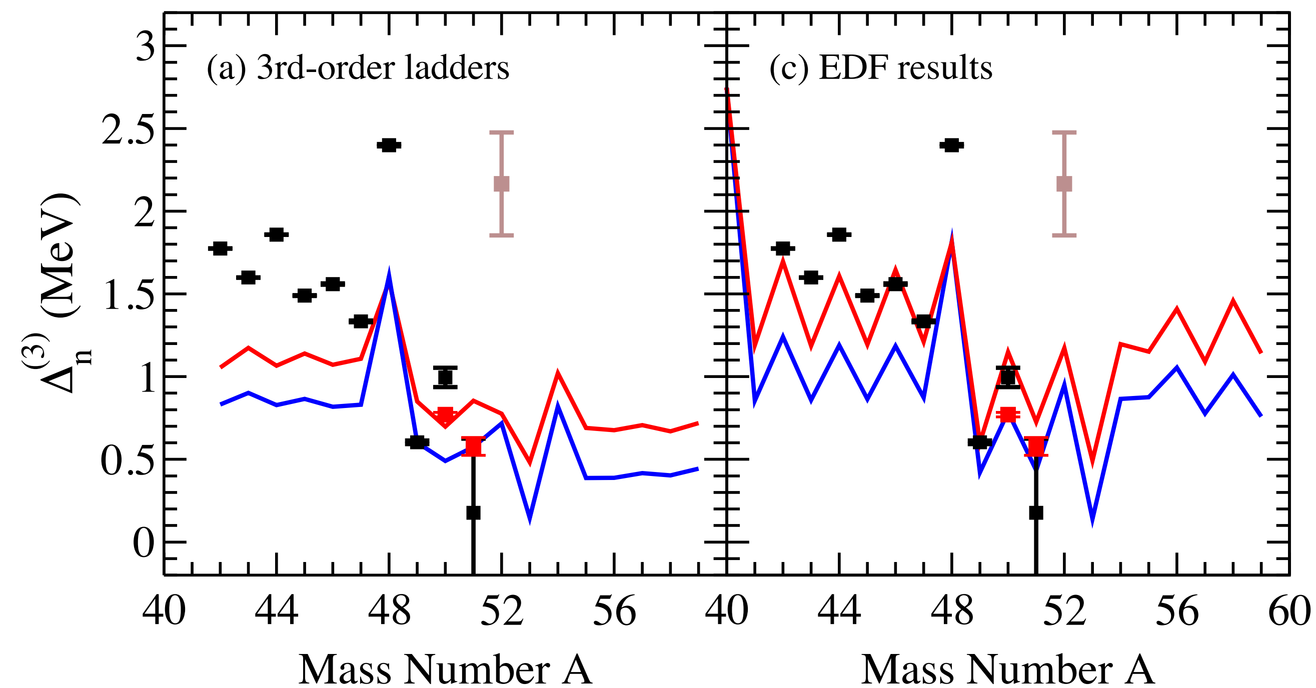


➠ Second order and 3NF necessary to invert the staggering

Pairing gaps

✪ Comparison with other microscopic SM and EDFs





[Holt, Menéndez, Schwenk 2013]

[Lesinski, Hebeler, Duguet, Schwenk 2012]

➟ General agreement with other methods

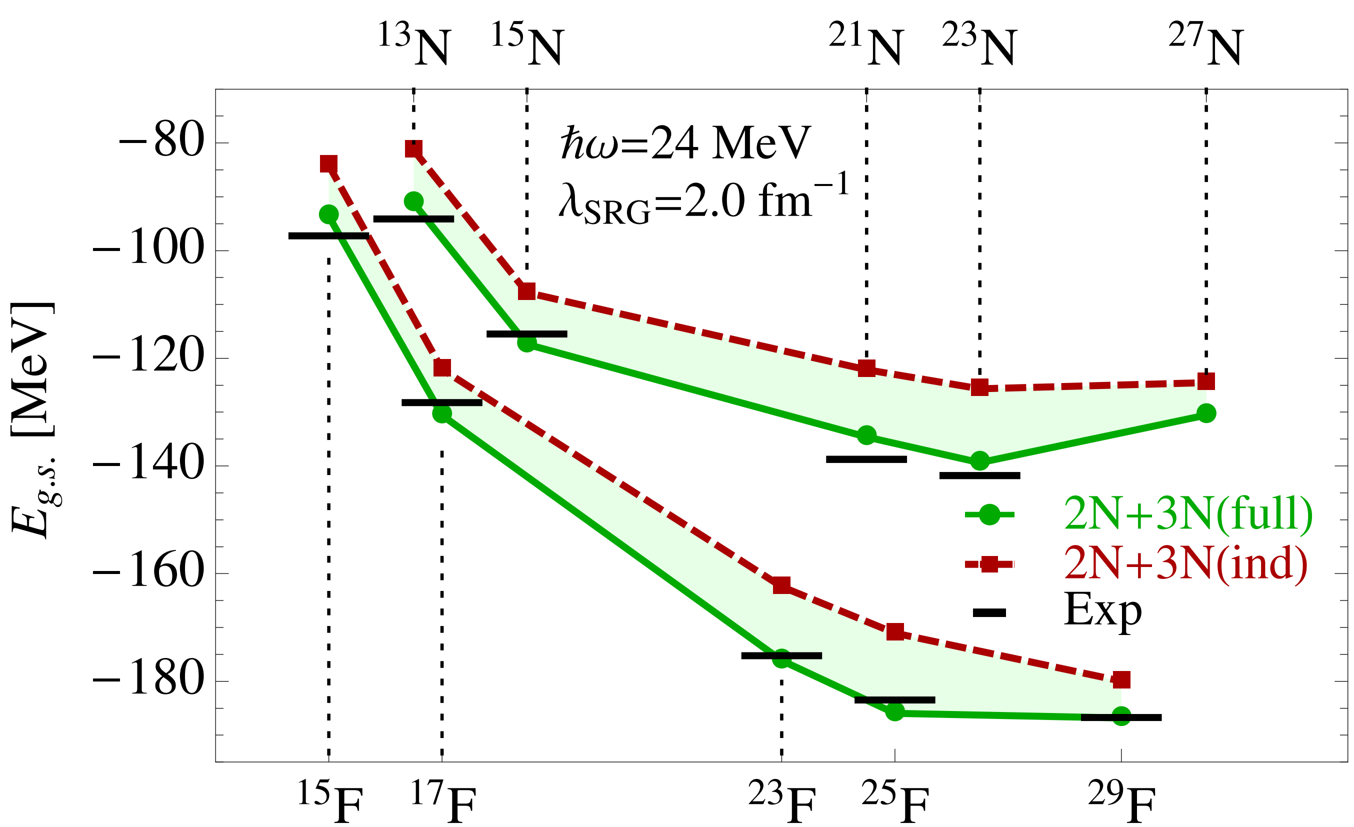
➟ Initial 3NF increase the gaps with respect to NN + induced 3NF

Benchmarks and chiral EFT interactions

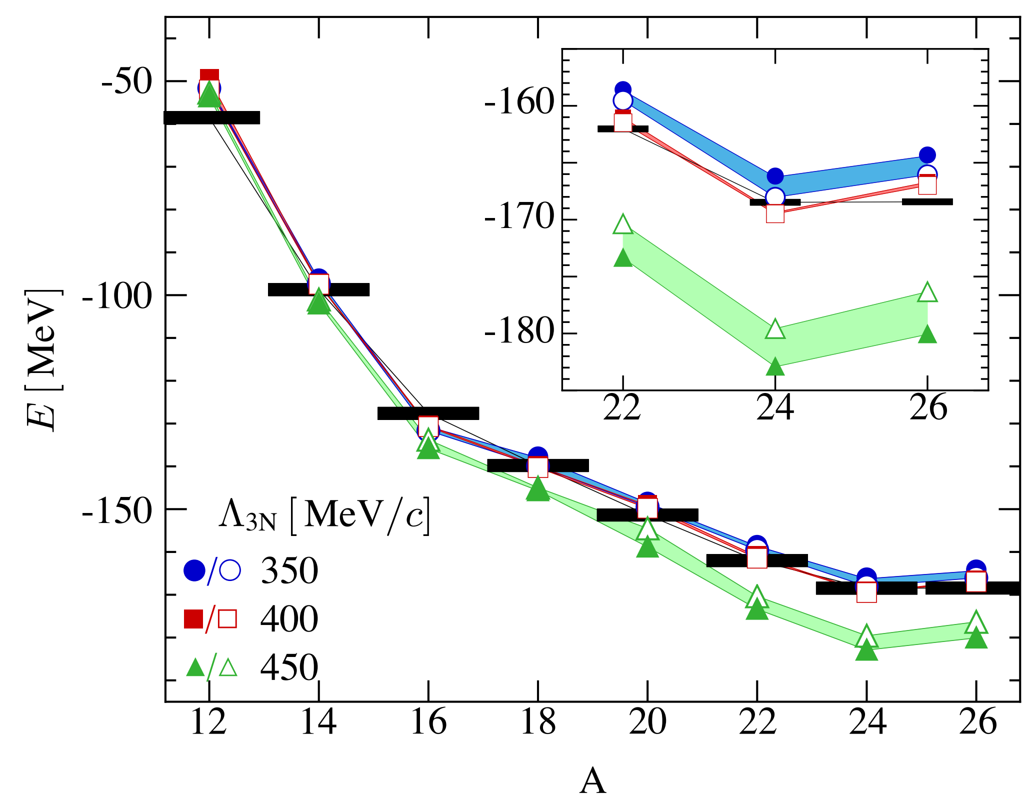
- ✪ *Ab initio* calculations as a test for chiral EFT interactions

- ✪ Different approaches agree in O and Ca chains

    ➟ Current chiral NN+3N forces overbind medium/heavy-mass nuclei



[Cipollone, Barbieri, Navrátil, 2013]



[Hergert *et al.*, 2013]

Spectral strength distribution

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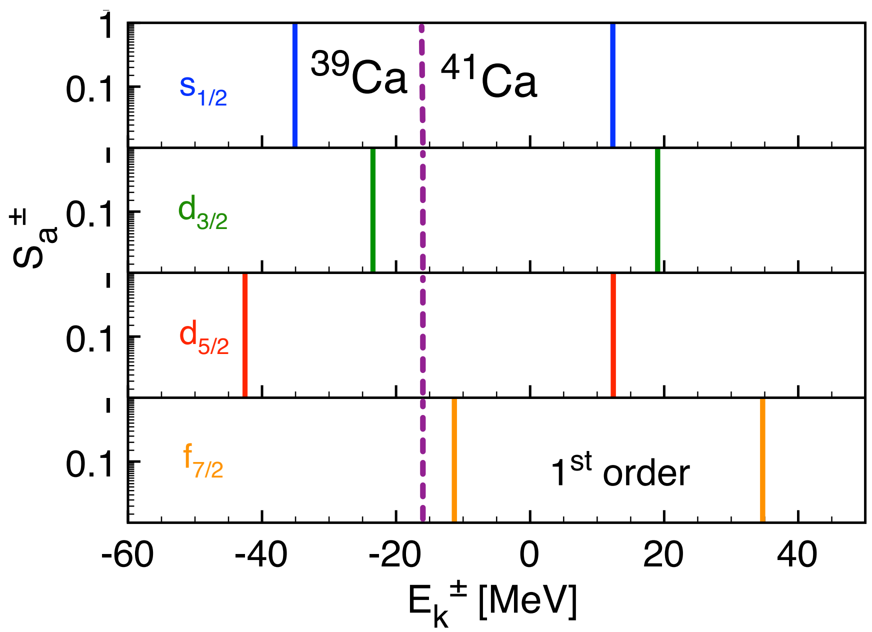
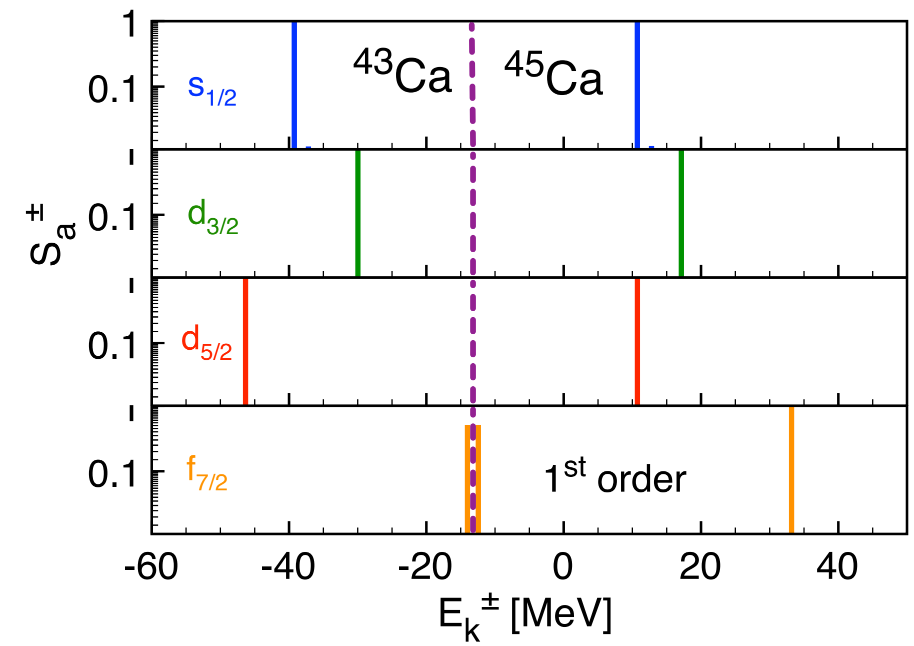
Dyson 1st order (HF)



Gorkov 1st order (HFB)

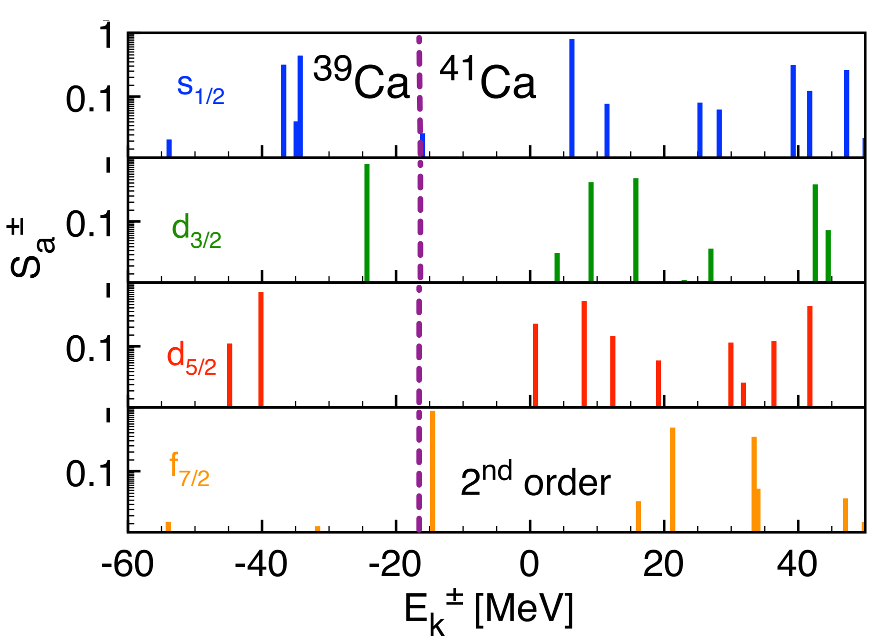


Fragmentation

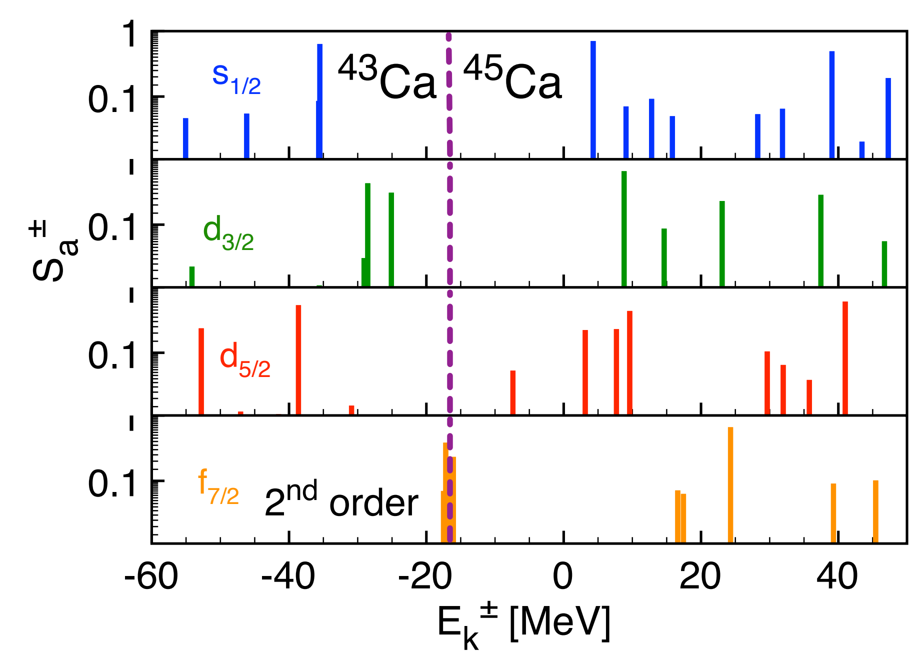
Static pairing

Dynamical fluctuations

Dyson 2nd order

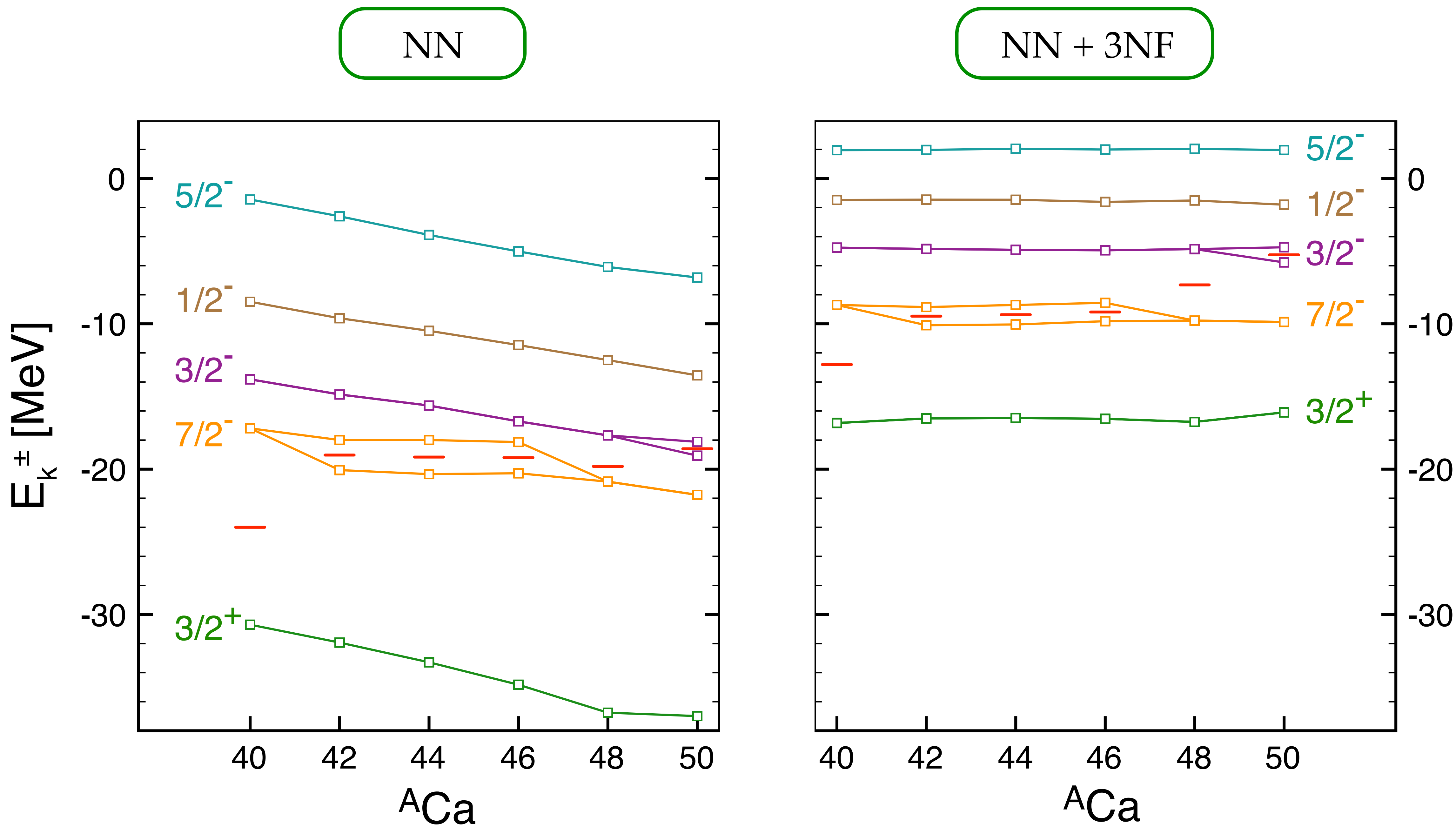


Gorkov 2nd order



Shell structure evolution

✪ One-neutron separation energies



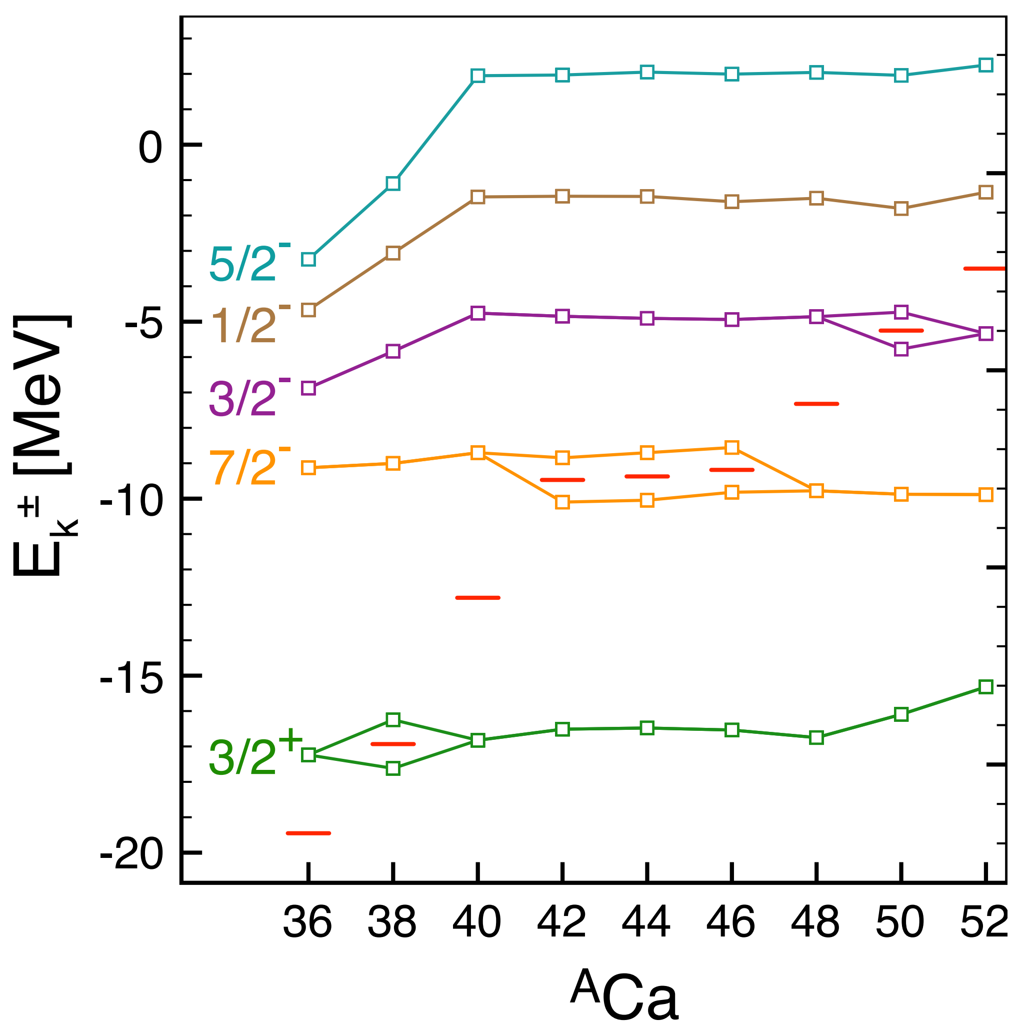
Shell structure evolution

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

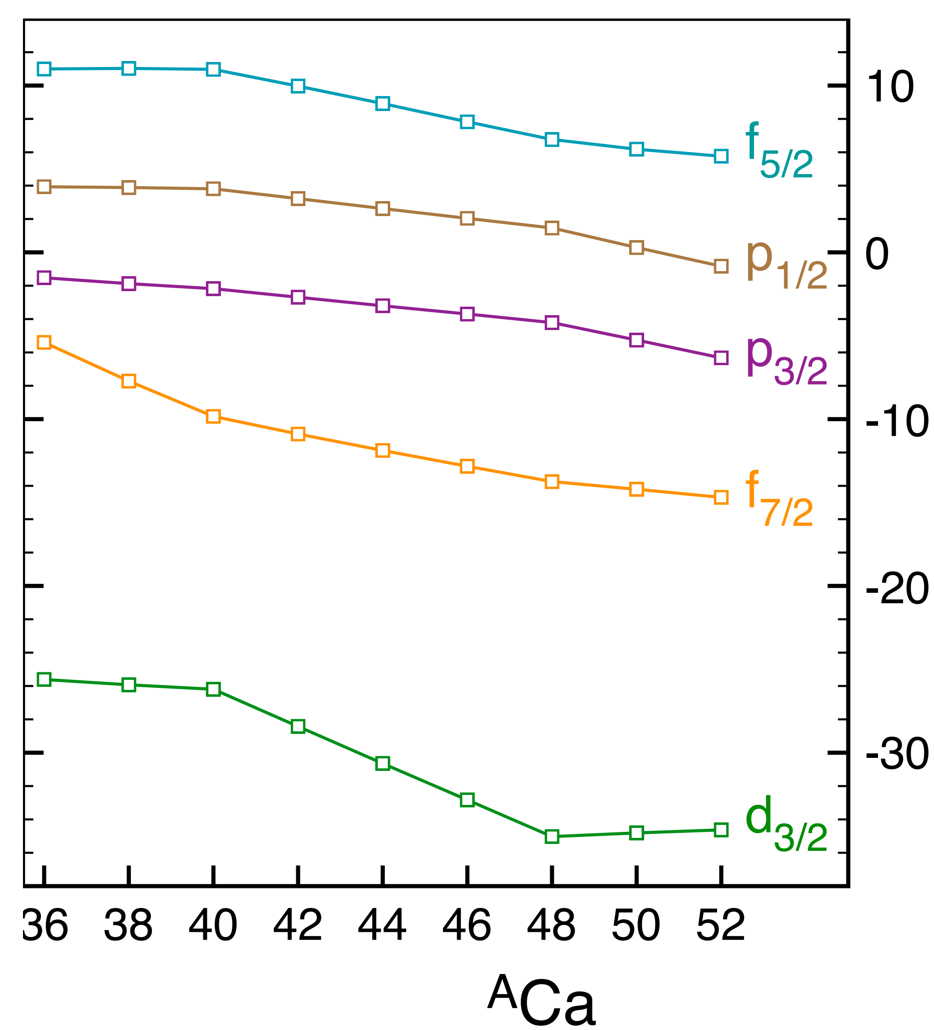
$$\epsilon_a^{cent} \equiv h_{ab}^{cent}\,\delta_{ab} = t_{aa} + \sum_{cd} \bar{V}^{NN}_{acad}\,\rho^{[1]}_{dc} + \sum_{cdef} \bar{V}^{NNN}_{acdaef}\,\rho^{[2]}_{efcd} \equiv \sum_k \mathcal{S}_k^{+a} E_k^{+} + \sum_k \mathcal{S}_k^{-a} E_k^{-}$$

[Baranger 1970, Duguet and Hagen 2011]

Separation energies

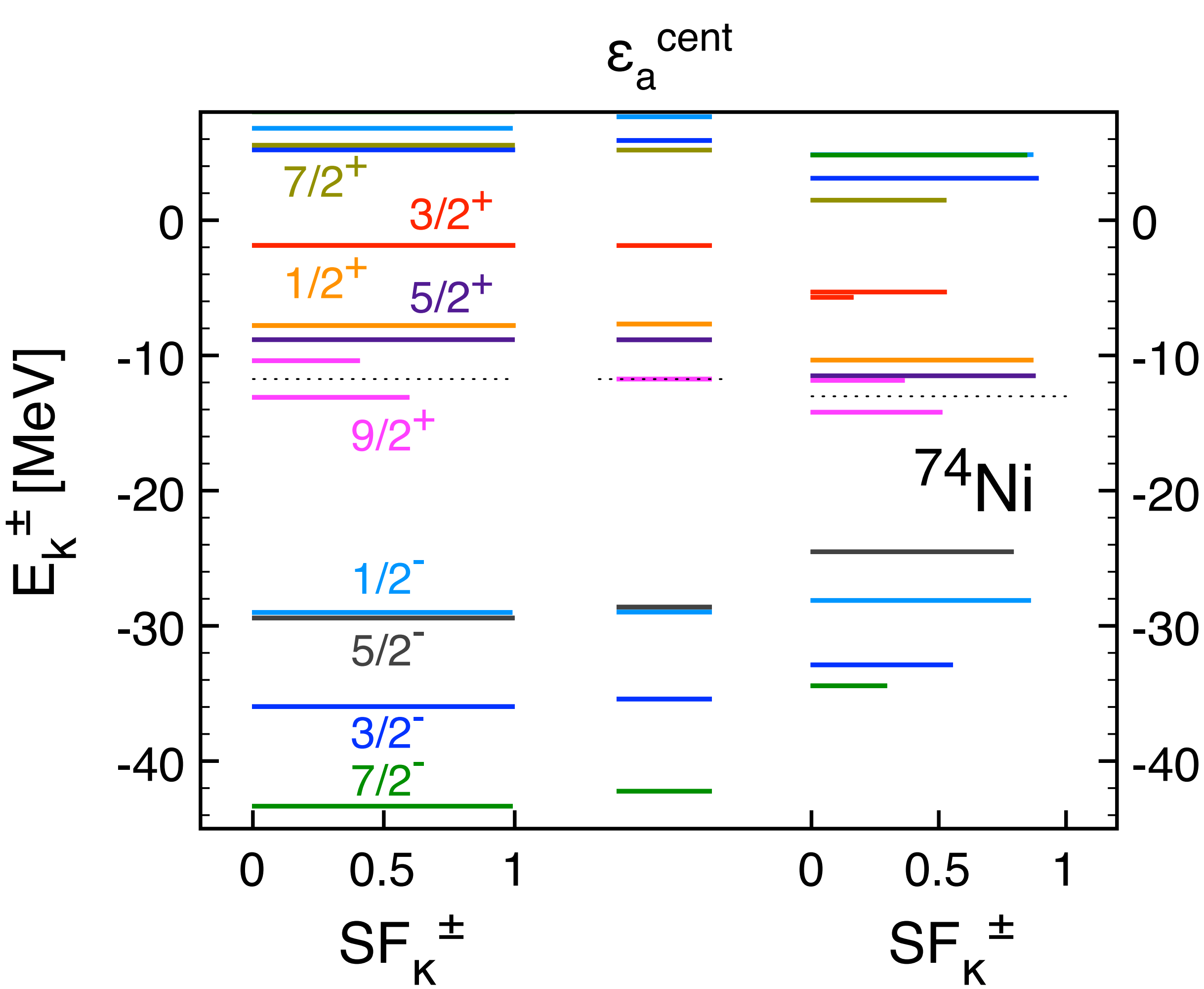


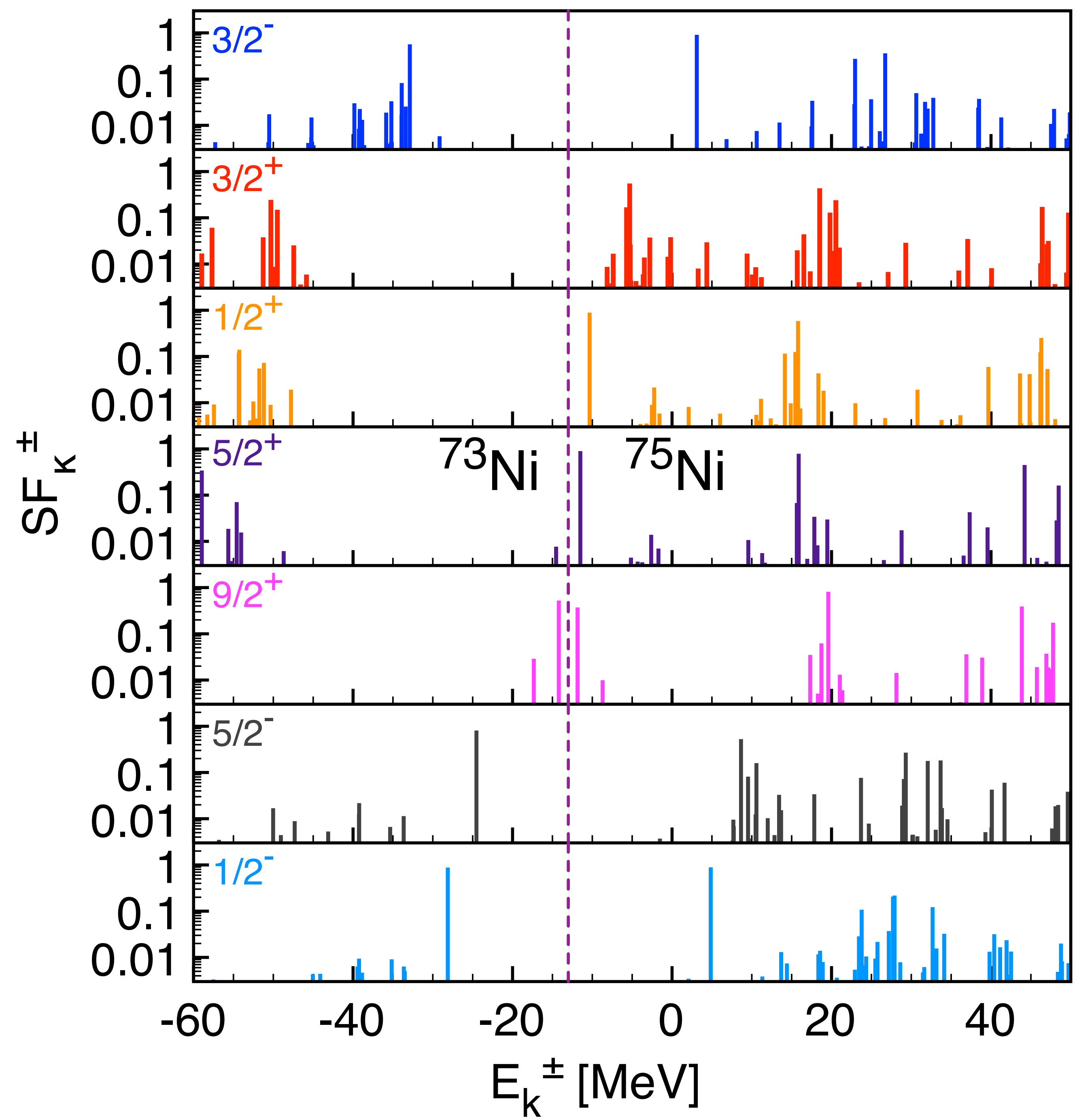
Centroids



Towards medium/heavy nuclei

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





Conclusions and outlook

✪ Gorkov-Green's functions:

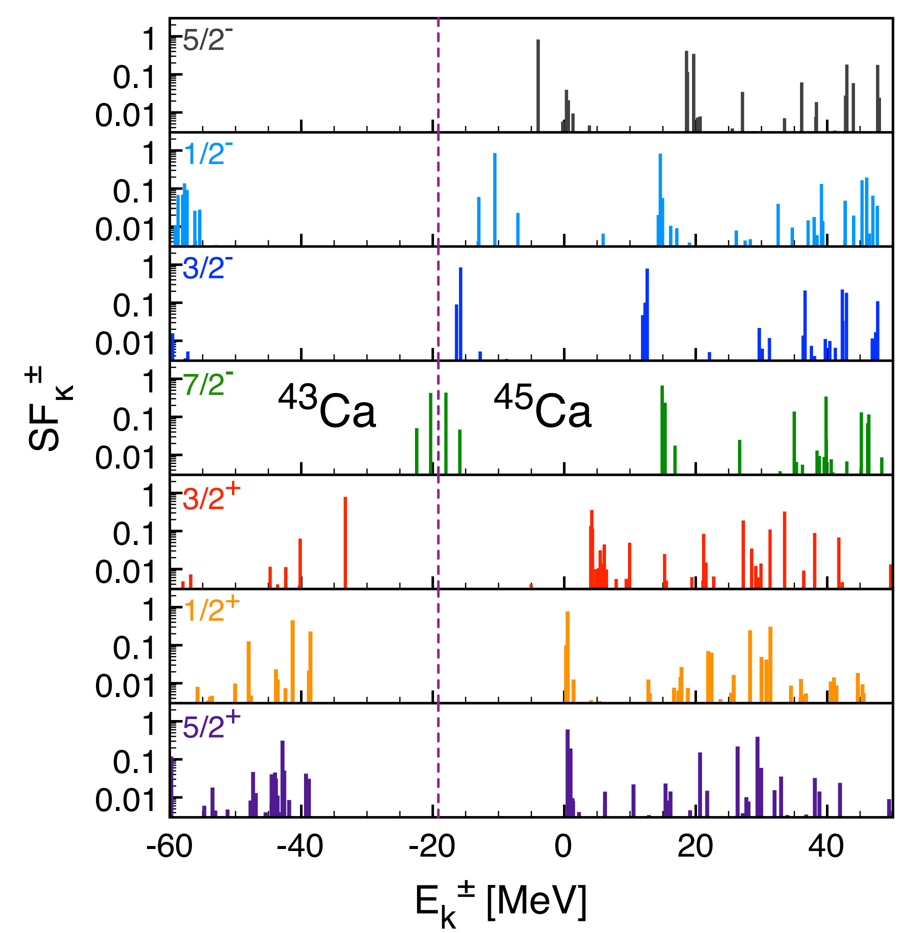
➟ Manageable route to (near) degenerate systems

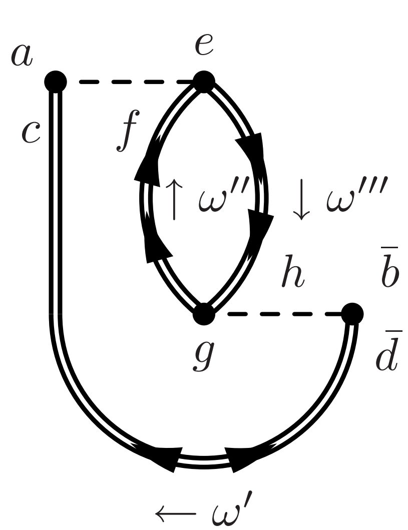
➟ *Ab initio* description of medium-mass chains

➟ 2NF + 3NF: towards predictive calculations

➟ Energies: quantitative agreement

➟ Spectra: study of shell structure evolution





✪ Improvement of the self-energy expansion

✪ Proper coupling to the continuum

✪ Formulation of particle-number restored Gorkov theory

✪ Towards consistent description of structure and reactions

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