Ab initio calculations as benchmarks for nuclear DFT

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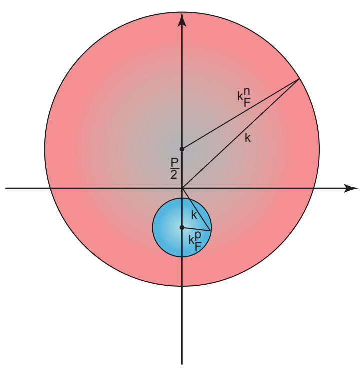
EMMI

Vittorio Somà (TU Darmstadt & EMMI)

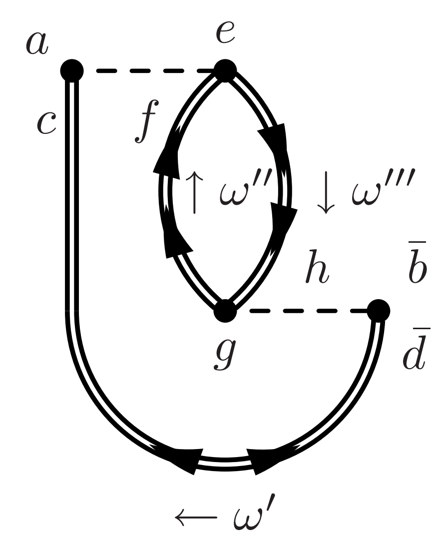
Nuclear matter:

- Drischler, Somà, Schwenk, *in preparation*



Nuclei:

- 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*



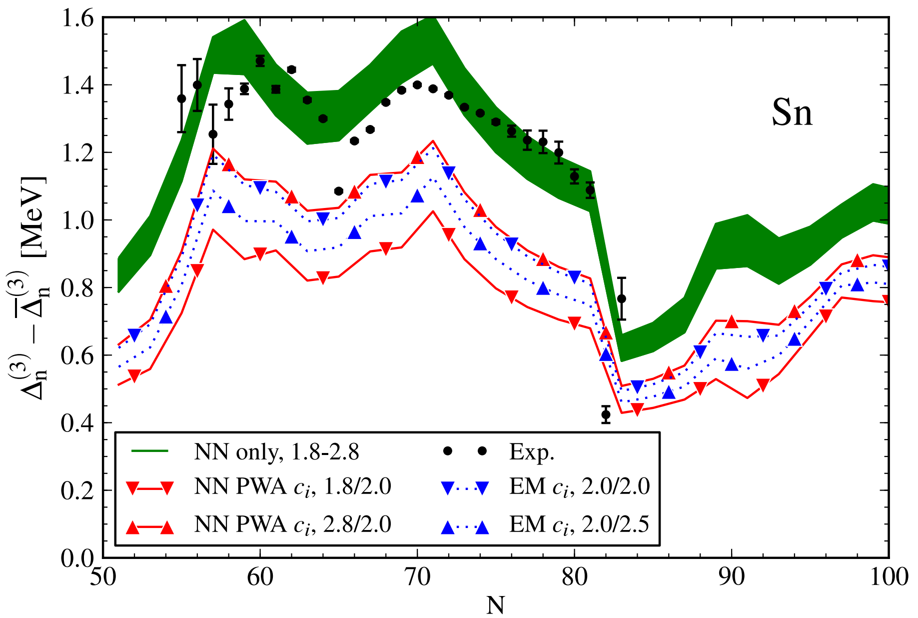
EMMI workshop, GSI
21 March 2013

Ab initio standpoint

- Connection with underlying inter-nucleon interactions
  - ➟ Microscopic perspective on new phenomena
- Predictive power
  - ➟ Crucial for exotic systems
  - ➟ Theoretical error estimates possible (and mandatory)
- Towards a more consistent description of structure and reactions
  - ➟ Crucial for interpretation of new experiments
- Provide benchmarks for other approaches
  - ➟ Important in the extension of traditional models to the neutron-rich sector

Ab initio methods and nuclear EDFs

- Towards *ab initio* EDFs
  - ➡ Density matrix expansion [Gebremariam, Duguet, Bogner 2010]
  - ➡ Low-momentum interactions in the pairing channel [Lesinski *et al.* 2011]



- Guidance for extensions and improvements of EDFs
  - ➡ UNEDF
- *Ab initio* method should share the same features of the EDF
  - ➡ E.g. symmetry breaking (and restoration)

Advances in the modeling of nuclear forces

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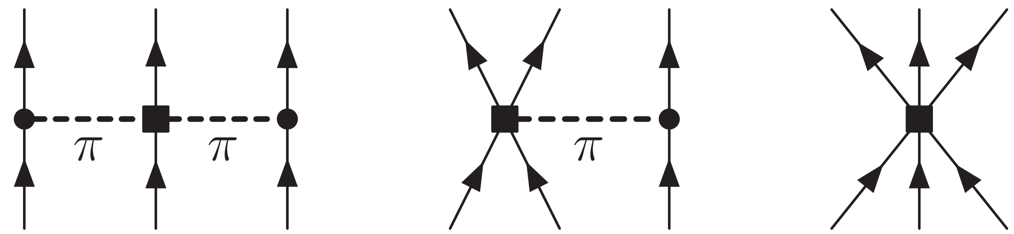
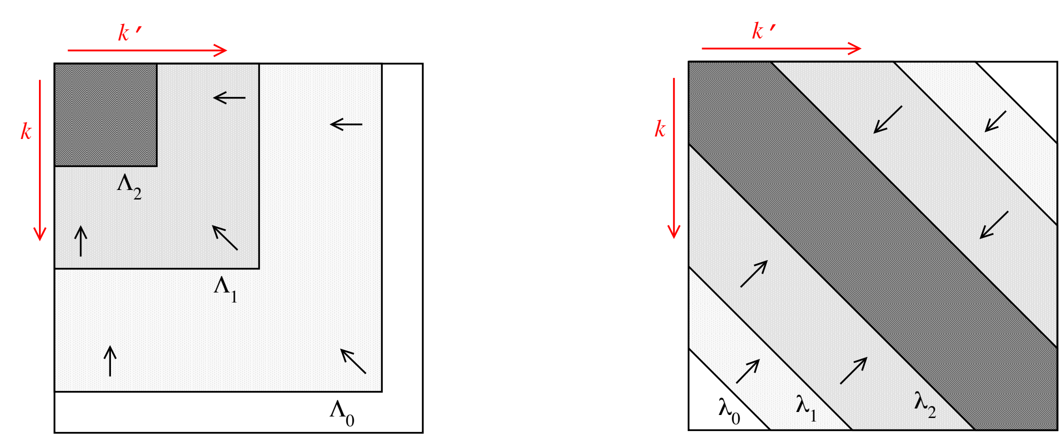
- Nuclear interactions from chiral EFT
  - ➟ Consistent many-body forces
  - ➟ A way to quantify theoretical errors



- Renormalization group techniques for NN and 3N forces
  - ➟ Many-body problem more perturbative



Estimation of theoretical errors

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✳ Crucial for benchmarking and extrapolations to neutron-rich sector

	Asymmetric matter	Medium-mass nuclei
1) Interaction	✔	✘
2) Many-body expansion	✘	✘
3) Model space truncation	✔	✔
4) Numerical algorithms	✔	✔

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Asymmetric nuclear matter

Asymmetric nuclear matter

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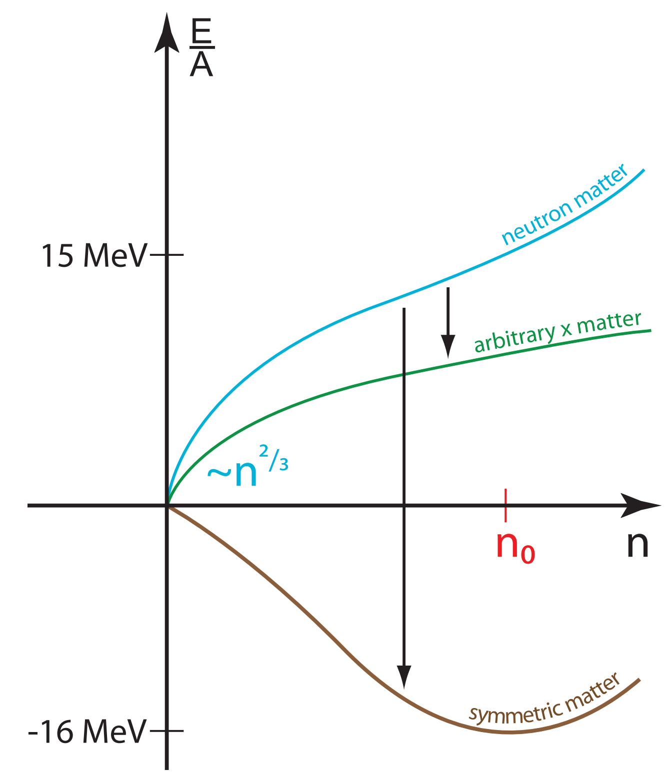
- Applications in astrophysical environments
  - ➟ Compact stars
  - ➟ Core-collapse supernovae

- Very few calculations with explicit isospin asymmetry
  - ➟ AFDMC [Fantoni *et al.* 2008]
    - NN only
  - ➟ SCGF [Frick *et al.* 2005]
    - NN only, finite temperature
  - ➟ BHF [Bombaci and Lombardo 1991, Zuo *et al.* 1999, Zuo 2012]



Asymmetric nuclear matter

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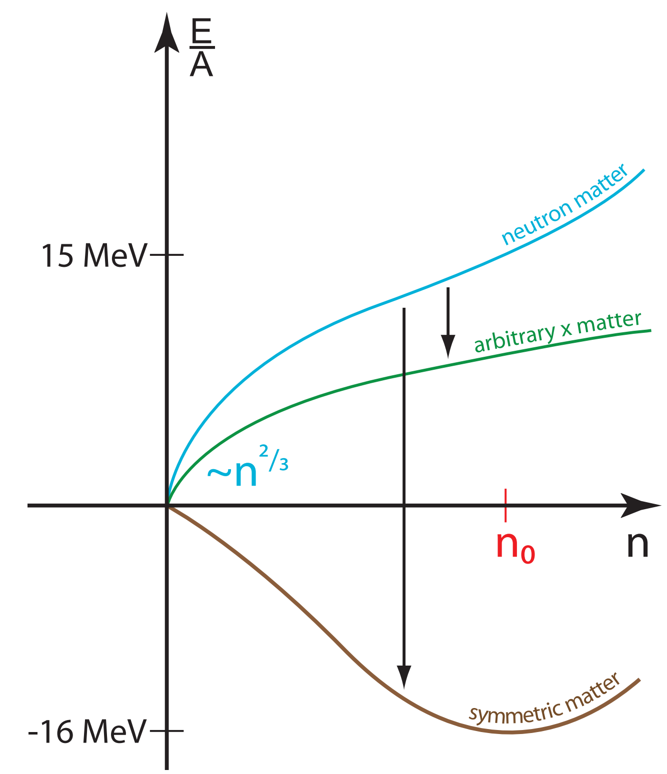


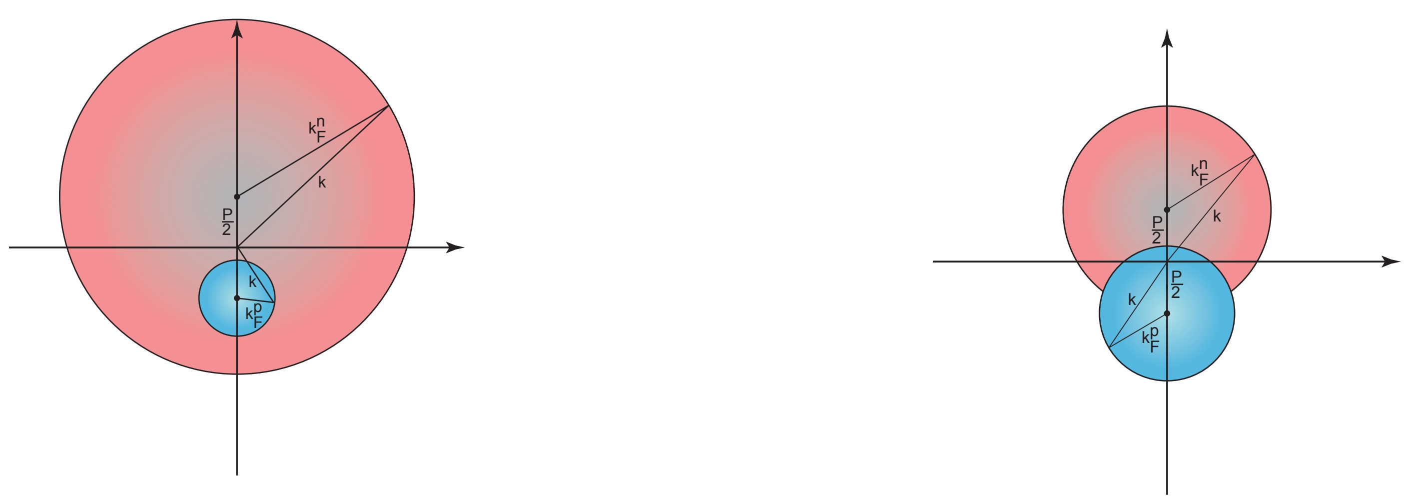
- Parabolic approximation

$$\frac{E(n,\beta)}{A} = \frac{E(n,\beta=0)}{A} + \beta^2\, E_{sym}(n) + \mathcal{O}(\beta^4)$$

where $\beta \equiv \dfrac{n_n - n_p}{n_n + n_p}$

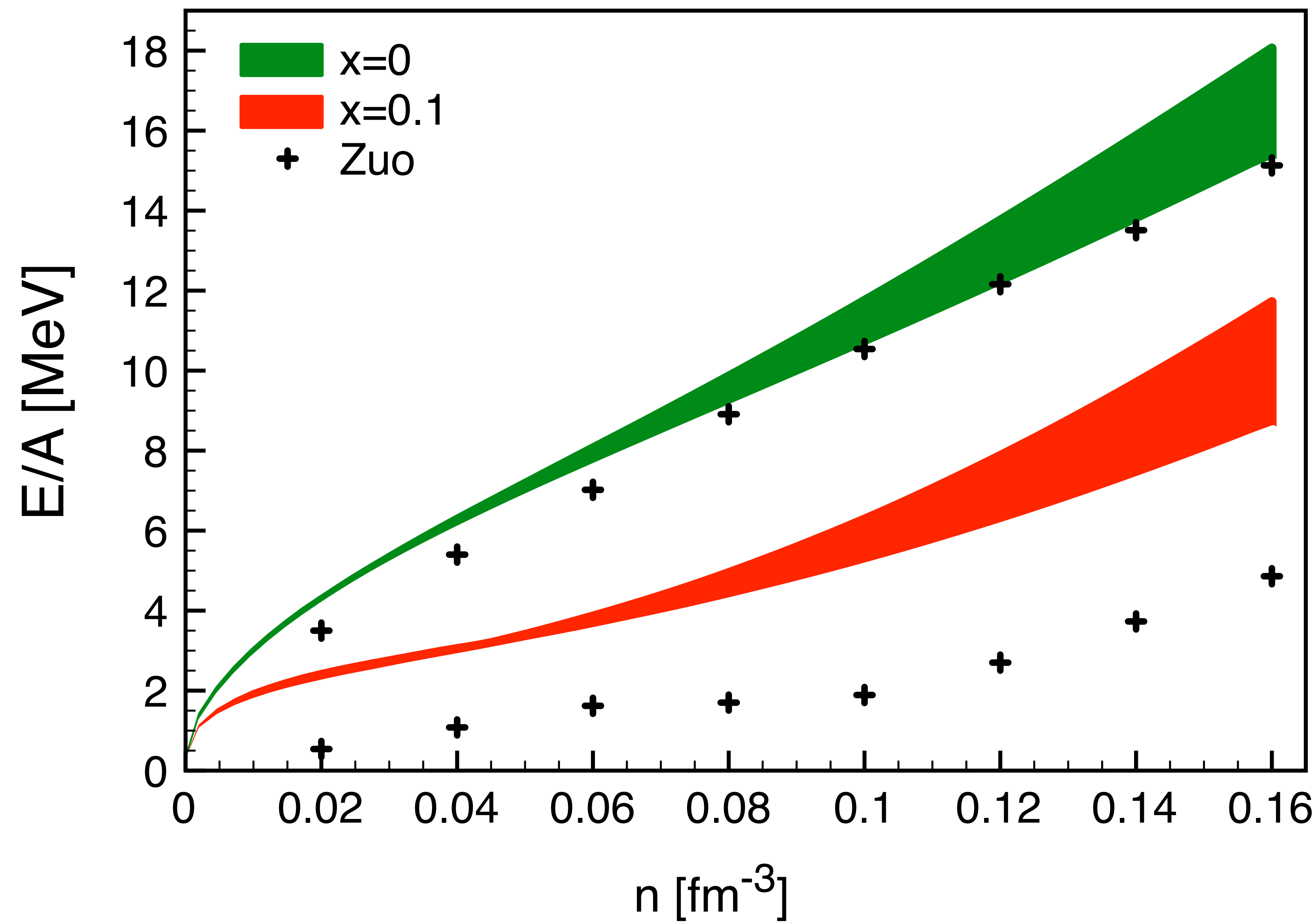
Calculation scheme

- MBPT(2)
  - chiral EFT N^3LO NN and N^2LO 3N interactions
  - NN evolved to low-momentum (see Gezerlis and Hebeler)
  - 3N forces at the HF level
  - Small x limit $x \equiv \frac{n_p}{n_n + n_p}$ → $V_{3N}\big|_x \approx V\big|_{nnn} + 3V\big|_{nnp}$
- Non-trivial integration over the two different Fermi spheres



[Drischler 2012]

Energy of asymmetric matter



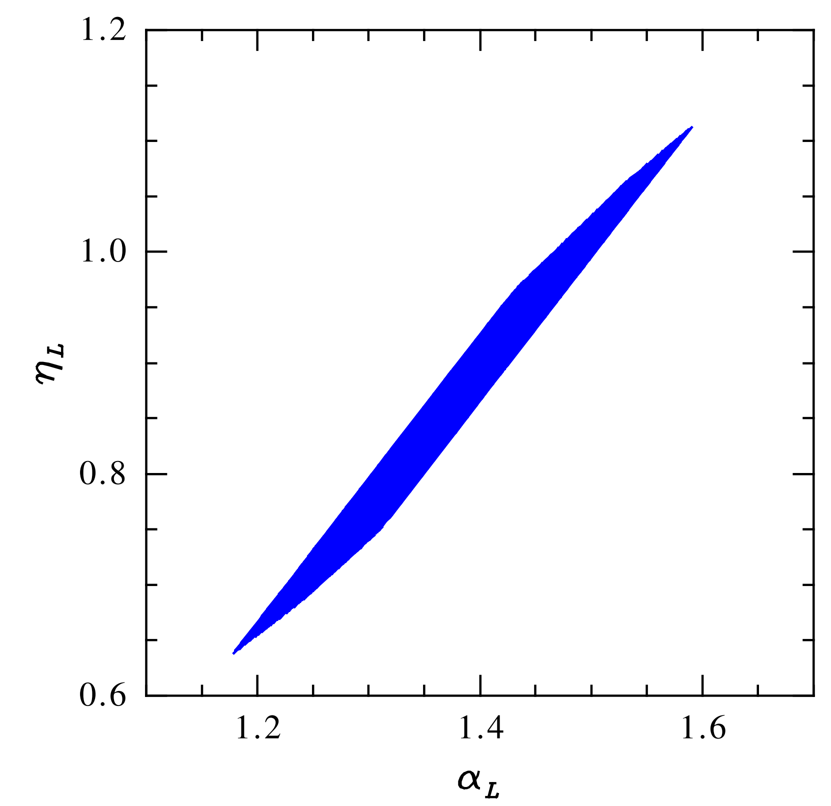
- NN interaction: chiral N^3LO evolved to low momentum [Entem and Machleidt 2003]
- Uncertainties: 7 sets of low-k (1.8-2.8 fm^{-1}) & 3N cutoffs

Quasi-parabolic expansion

- Expression for the energy per particle in asymmetric matter

  ➟ Kinetic energy + interpolation of interaction energy

$$\frac{E(\overline{n},x)}{A} = T_0 \Bigg[\frac{3}{5} \left(x^{\frac{5}{3}} + (1-x)^{\frac{5}{3}} \right) (2\overline{n})^{\frac{2}{3}} - \left((2\alpha - 4\alpha_L)\, x\, (1-x) + \alpha_L \right) \overline{n} + \left((2\eta - 4\eta_L)\, x\, (1-x) + \eta_L \right) \overline{n}^{\gamma} \Bigg]$$



[Hebeler, Lattimer, Pethick, Schwenk 2013]

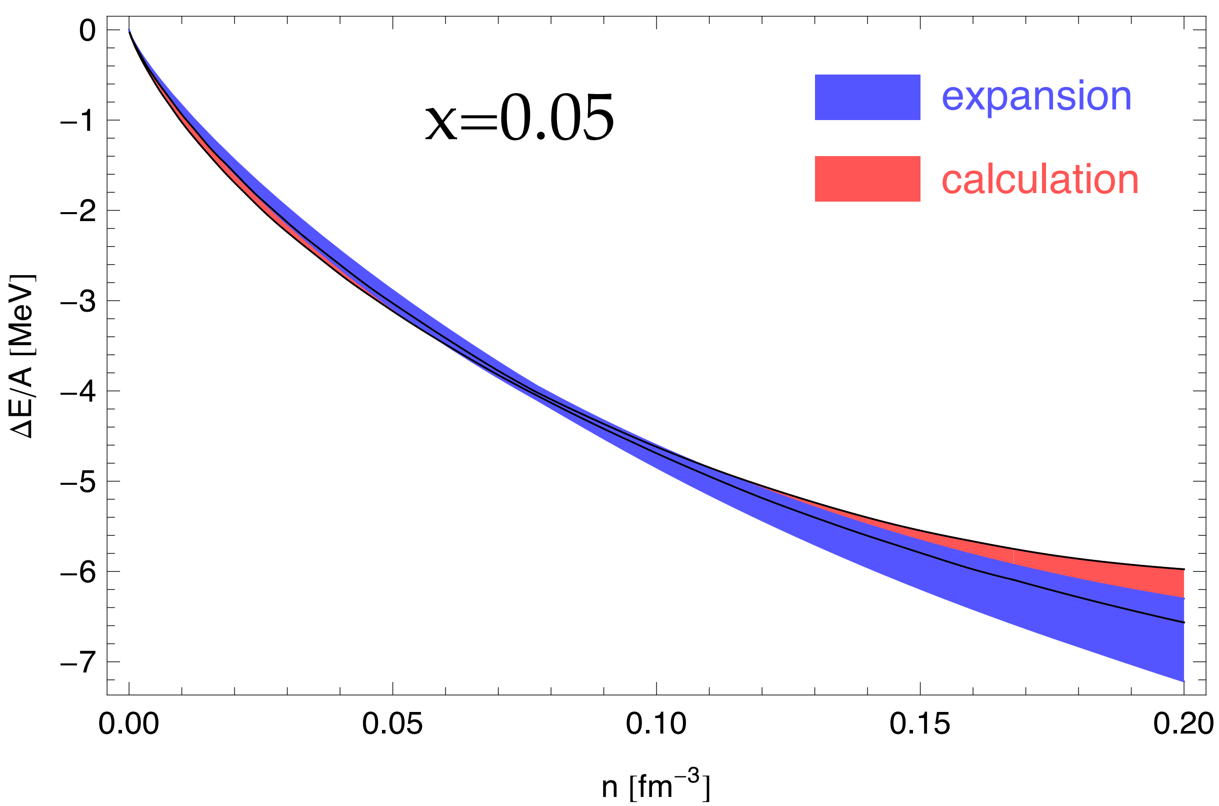
➟ Parameters determined from

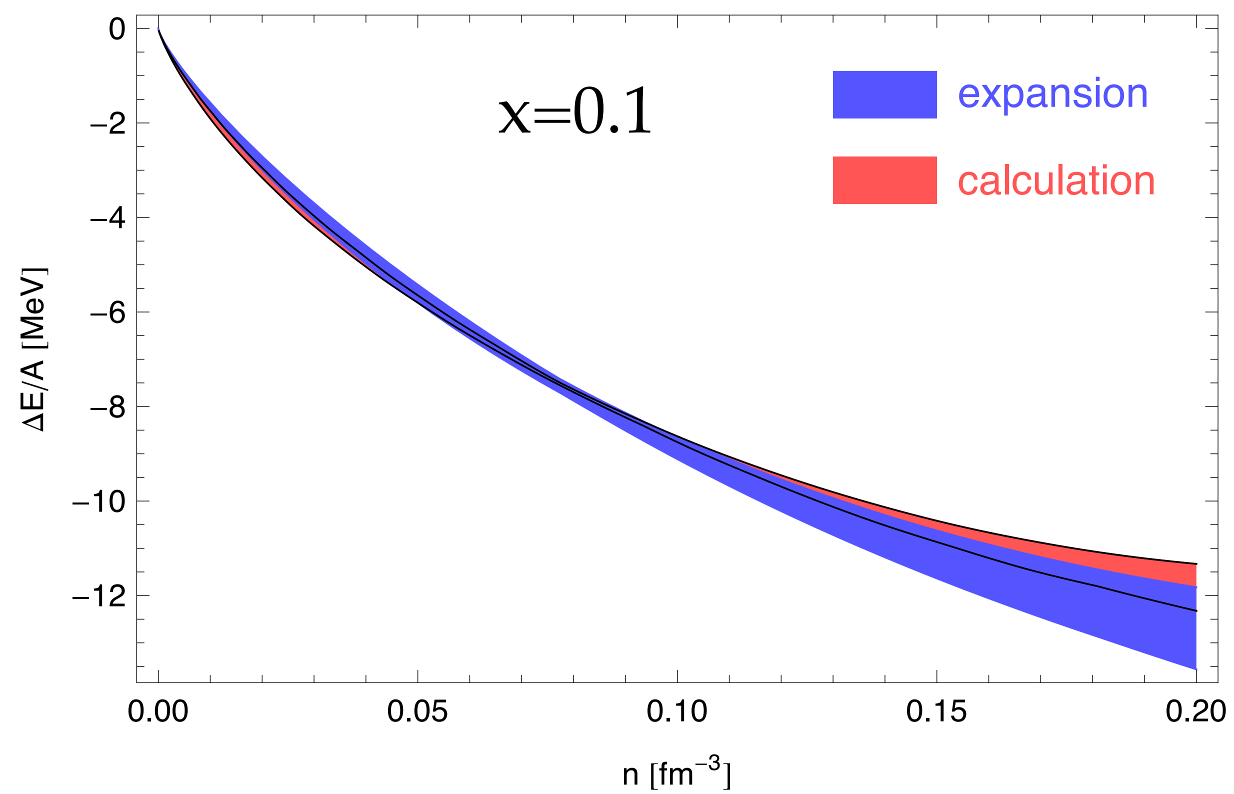
- saturation properties of symmetric matter
- neutron matter energy and pressure calculations

Validation of quasi-parabolic expansion

- Compare energy relative to pure neutron matter

$$\frac{\Delta E(n,x)}{A} = \frac{E(n,x)}{A} - \frac{E(n,x=0)}{A}$$





➟ Excellent agreement within uncertainties

➟ Possible improvements in the expansion

Conclusions and outlook (part I)

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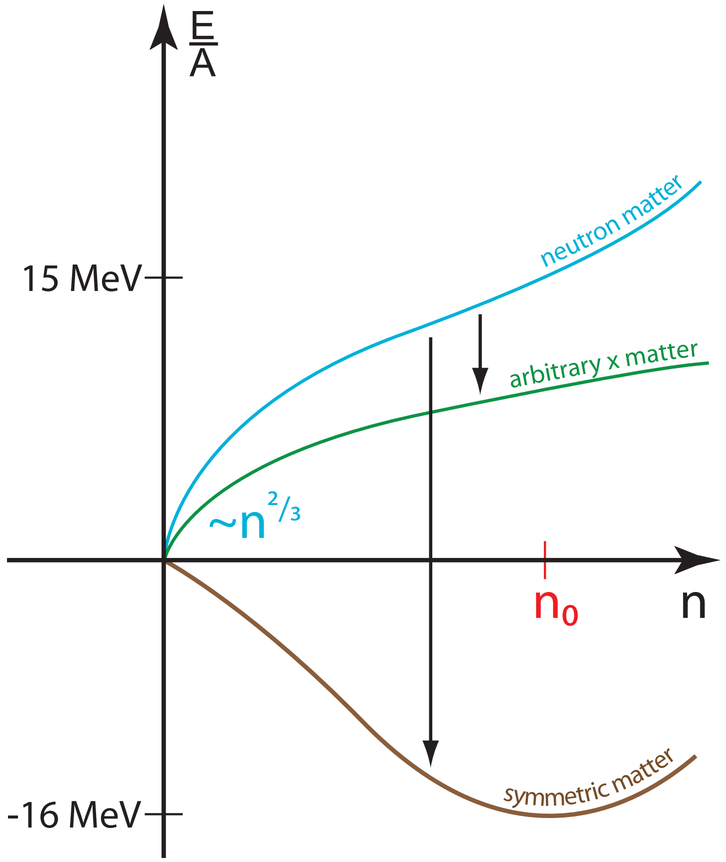
- First explicit calculation of asymmetric matter with chiral interactions
  - ➡ Constrain isospin dependence of nuclear EOS
  - ➡ Revisit parabolic approximation for small proton fractions

- Outlook
  - ➡ Improve many-body expansion
  - ➡ Use consistently evolved NN+3N interactions
  - ➡ Release small proton fraction approximation



Open-shell medium-mass nuclei

Advances in *ab initio* techniques

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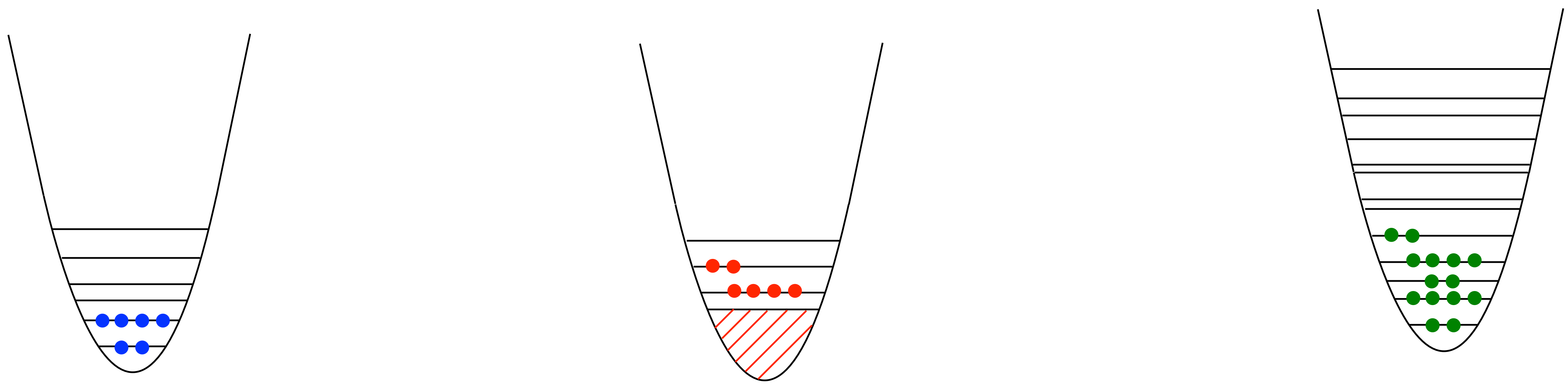
Light nuclei | Medium-mass nuclei | Medium-mass nuclei



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

Going open-shell: Gorkov's idea

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- Bogoliubov algebra + Green's function theory

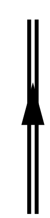
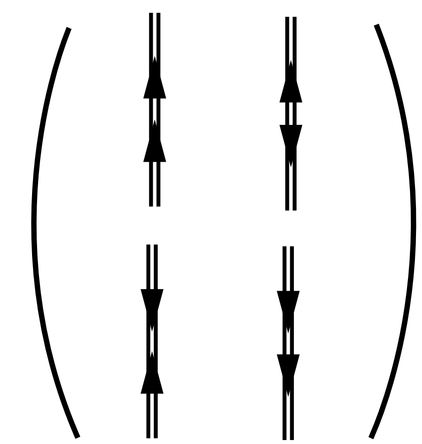
- Keep the simplicity of a single-reference

- Address explicitly the non-perturbative formation of Cooper pairs

  ➟ Formulate the expansion scheme around a Bogoliubov vacuum

  ➟ Breaking of particle-number conservation (eventually restored)

Going open-shell: Gorkov's formalism

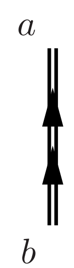
	Dyson	*Gorkov*
◦ Reference state	$\vert\psi_0^A\rangle$	$\vert\Psi_0\rangle \equiv \sum_A^{\text{even}} c_A \vert\psi_0^A\rangle$
◦ One-body propagator	$G_{ab} =$ 	$\mathbf{G}_{ab} = \begin{pmatrix} G_{ab}^{11} & G_{ab}^{12} \\ G_{ab}^{21} & G_{ab}^{22} \end{pmatrix} =$ 
◦ Hamiltonian	H	$\Omega = H - \mu A$
◦ G.S. energy	E_0^A	$\Omega_0 = \sum_{A'} \vert c_{A'}\vert^2 \, \Omega_0^{A'} \approx E_0^A - \mu A$

[Gorkov 1958]

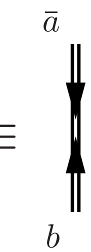
Gorkov equations

✺ Set of 4 Green's functions

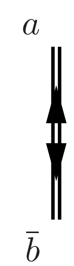
$$i\,G^{11}_{ab}(t,t') \equiv \langle \Psi_0 | T\left\{ a_a(t) a^\dagger_b(t') \right\} | \Psi_0 \rangle \equiv$$



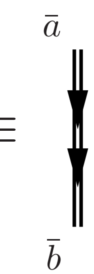
$$i\,G^{21}_{ab}(t,t') \equiv \langle \Psi_0 | T\left\{ \bar{a}^\dagger_a(t) a^\dagger_b(t') \right\} | \Psi_0 \rangle \equiv$$



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



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

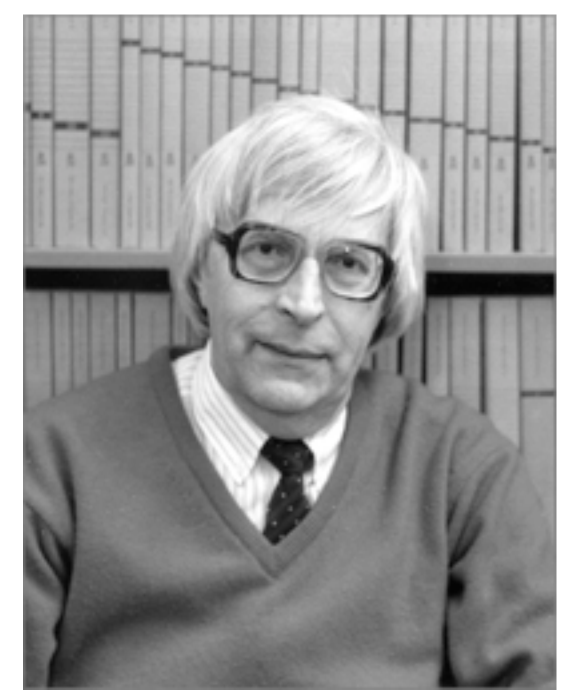


↓

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

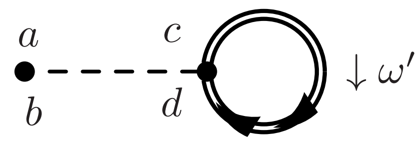
Gorkov equations

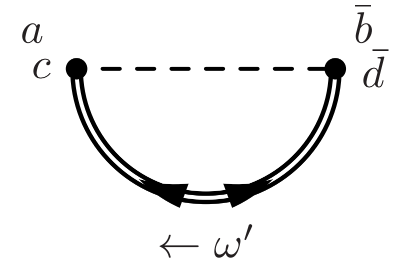
[Gorkov 1958]



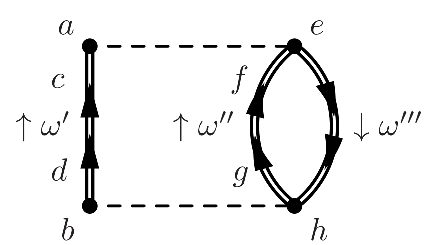
Self-energy expansion

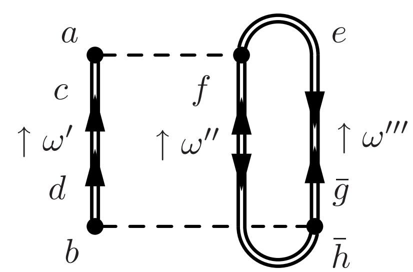
✺ 1st order ➟ energy-independent self-energy

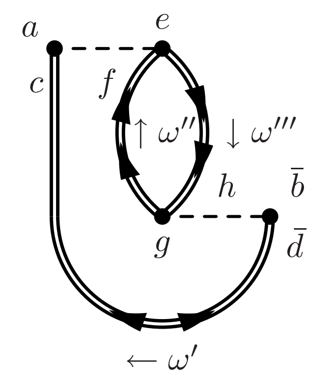
$\Sigma^{11\,(1)}_{ab} =$ 

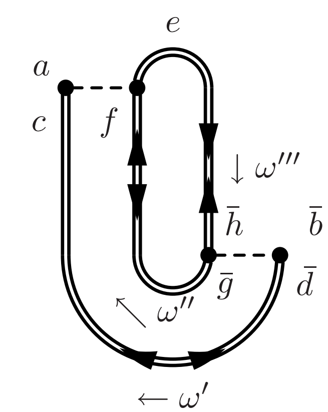
$\Sigma^{12\,(1)}_{ab} =$ 

✺ 2nd order ➟ energy-dependent self-energy

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

$+$ 

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

$+$ 

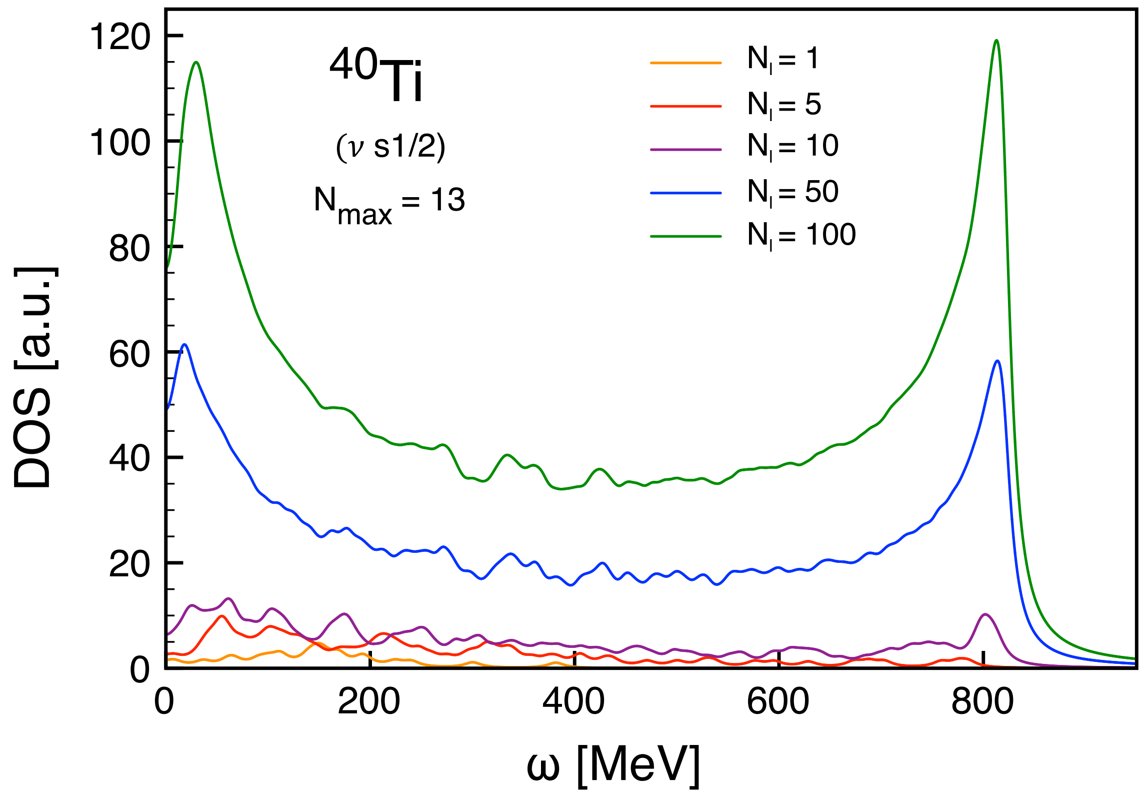
✺ Gorkov equations ⟶ energy *dependent* eigenvalue problem

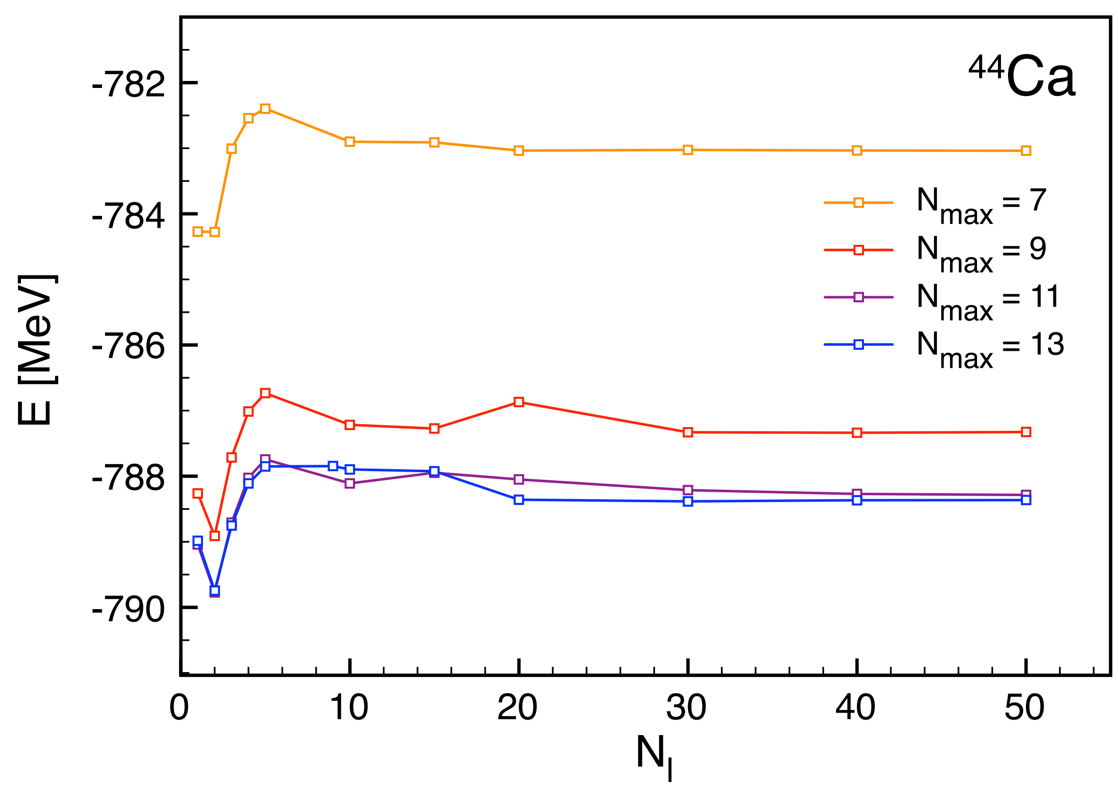
$$\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & -t_{ab} + \mu_{ab} + \Sigma^{22}_{ab}(\omega) \end{pmatrix}\Bigg|_{\omega_k} \begin{pmatrix} \mathcal{U}^k_b \\ \mathcal{V}^k_b \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k_a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

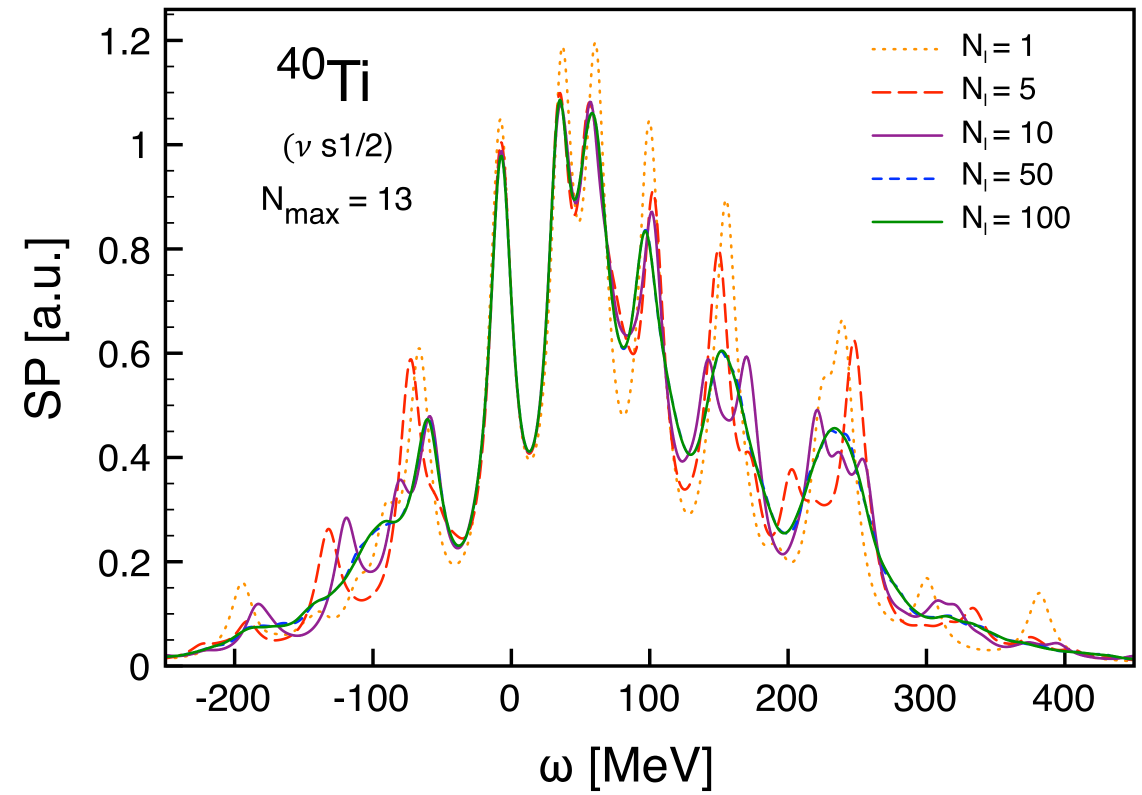
$$\mathcal{U}^{k*}_a \equiv \langle \Psi_k | \bar{a}^\dagger_a | \Psi_0 \rangle$$
$$\mathcal{V}^{k*}_a \equiv \langle \Psi_k | a_a | \Psi_0 \rangle$$

Krylov projection

- ➟ Krylov projection of Gorkov's matrix
- ➟ Lanczos-like algorithm
- ➟ Conserves moments of spectral functions
- ➟ Results become independent of N_l



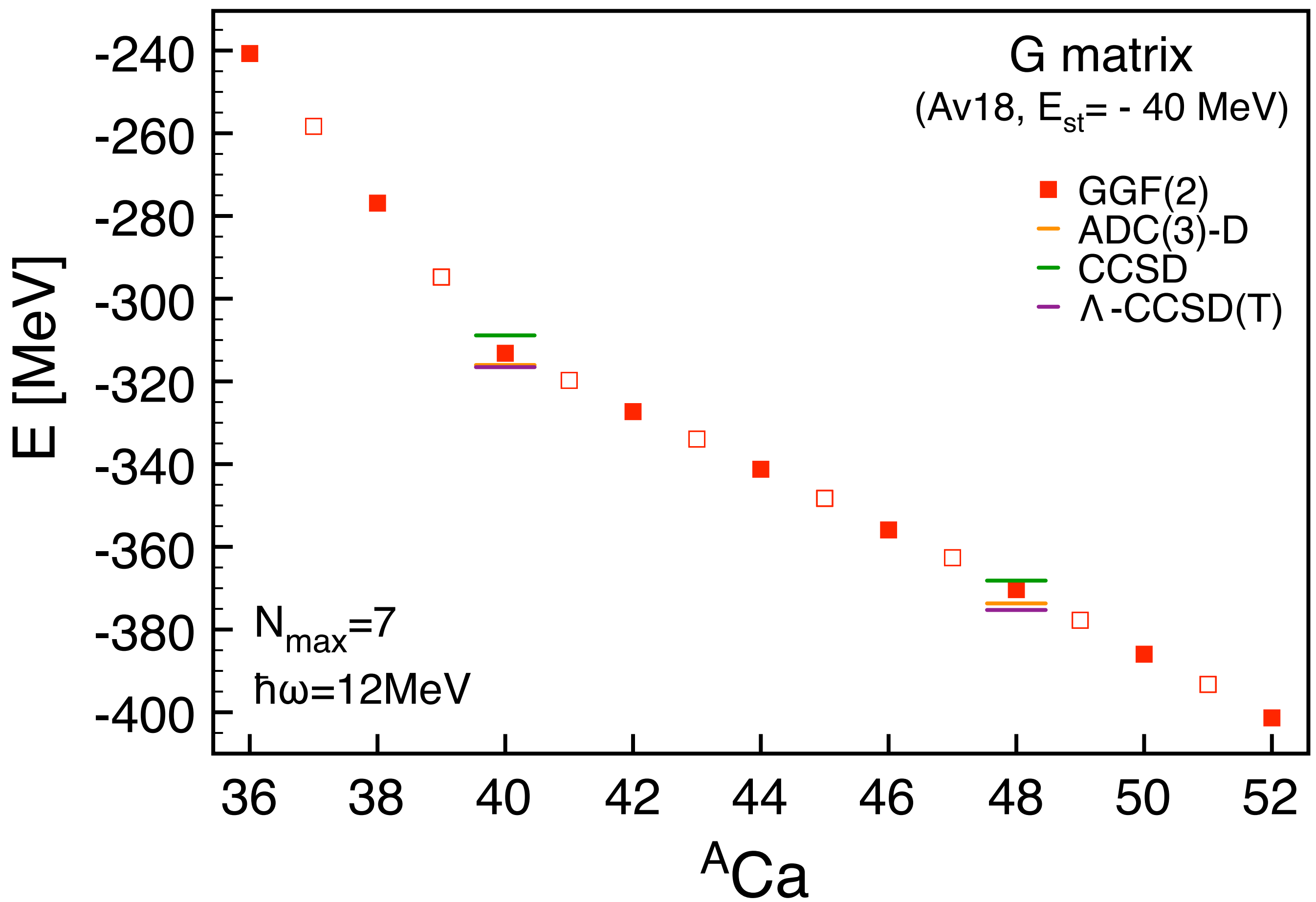




Benchmark with coupled cluster method

✷ Energy from Galitskii-Koltun sum rule

$$E_0^{\mathrm{A}} = \frac{1}{4\pi i} \int_{C\uparrow} d\omega \, \mathrm{Tr}_{\mathcal{H}_1} [\mathbf{G}^{11}(\omega)[\mathbf{T} + (\mu + \omega)\,\mathbf{1}]]$$



➟ GGF and CC quantitatively similar

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

(CC results courtesy of G. Hagen)

Towards medium/heavy open-shell

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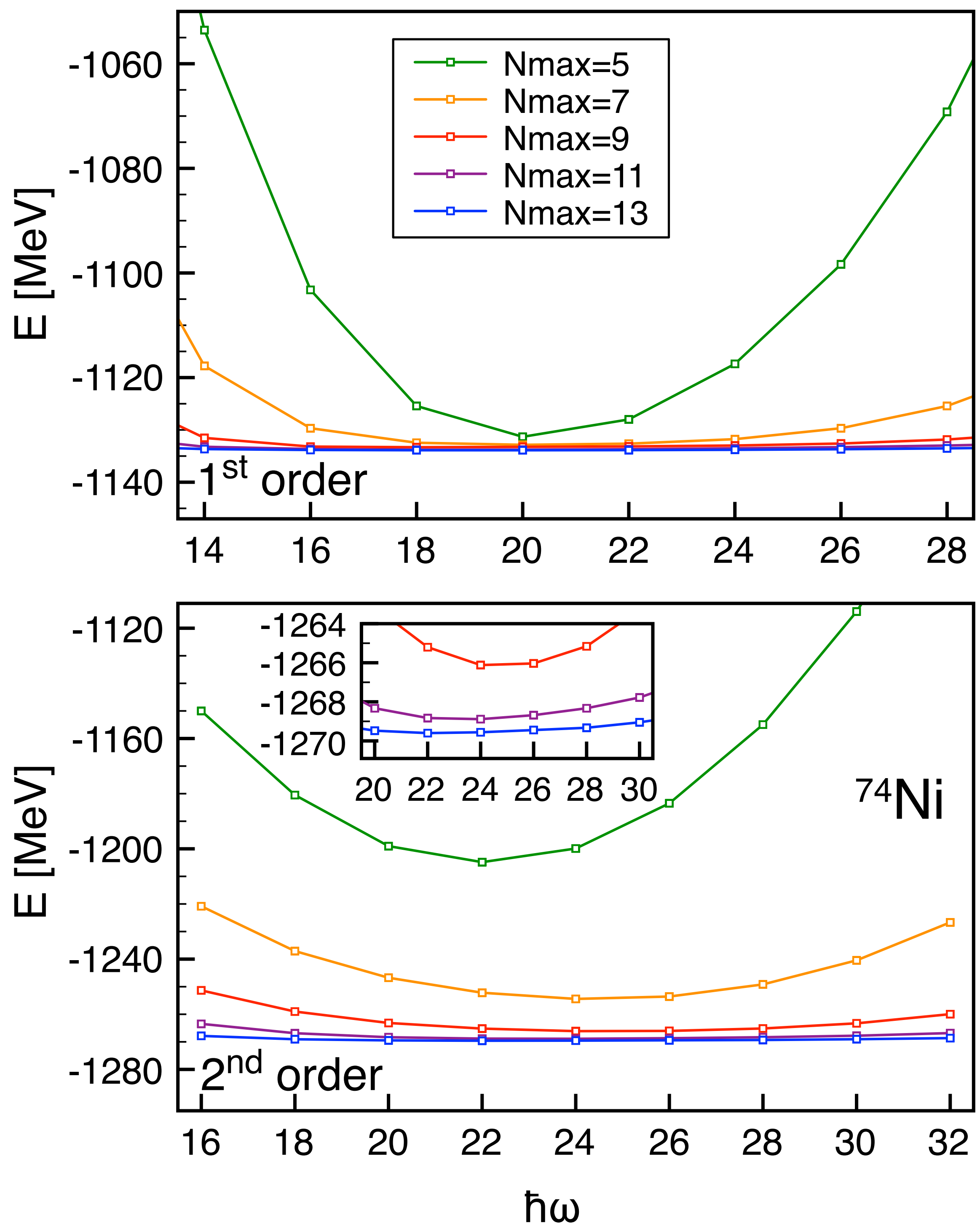
- ^{74}Ni



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

[Entem and Machleidt 2003]

➟ Very good convergence

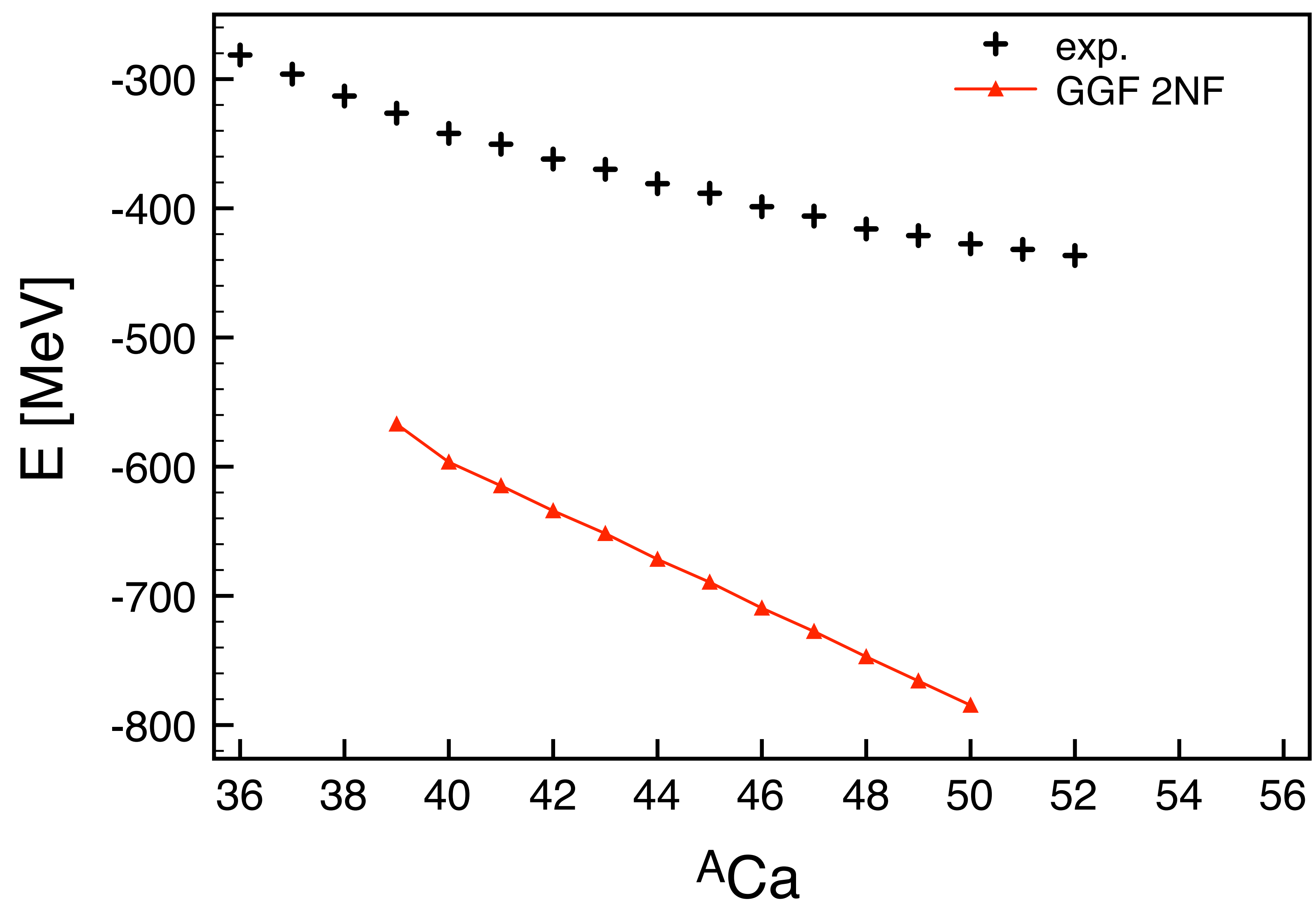
➟ From N=13 to N=11 → 200 keV

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

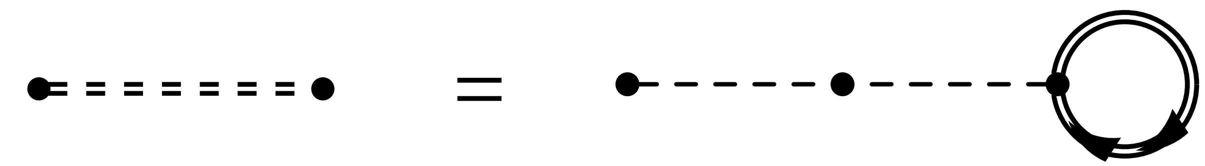
- NN only
  - ➟ Systematic along isotopic/isotonic becomes available
  - ➟ Overbinding (increasing with A): need for three-body forces



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

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

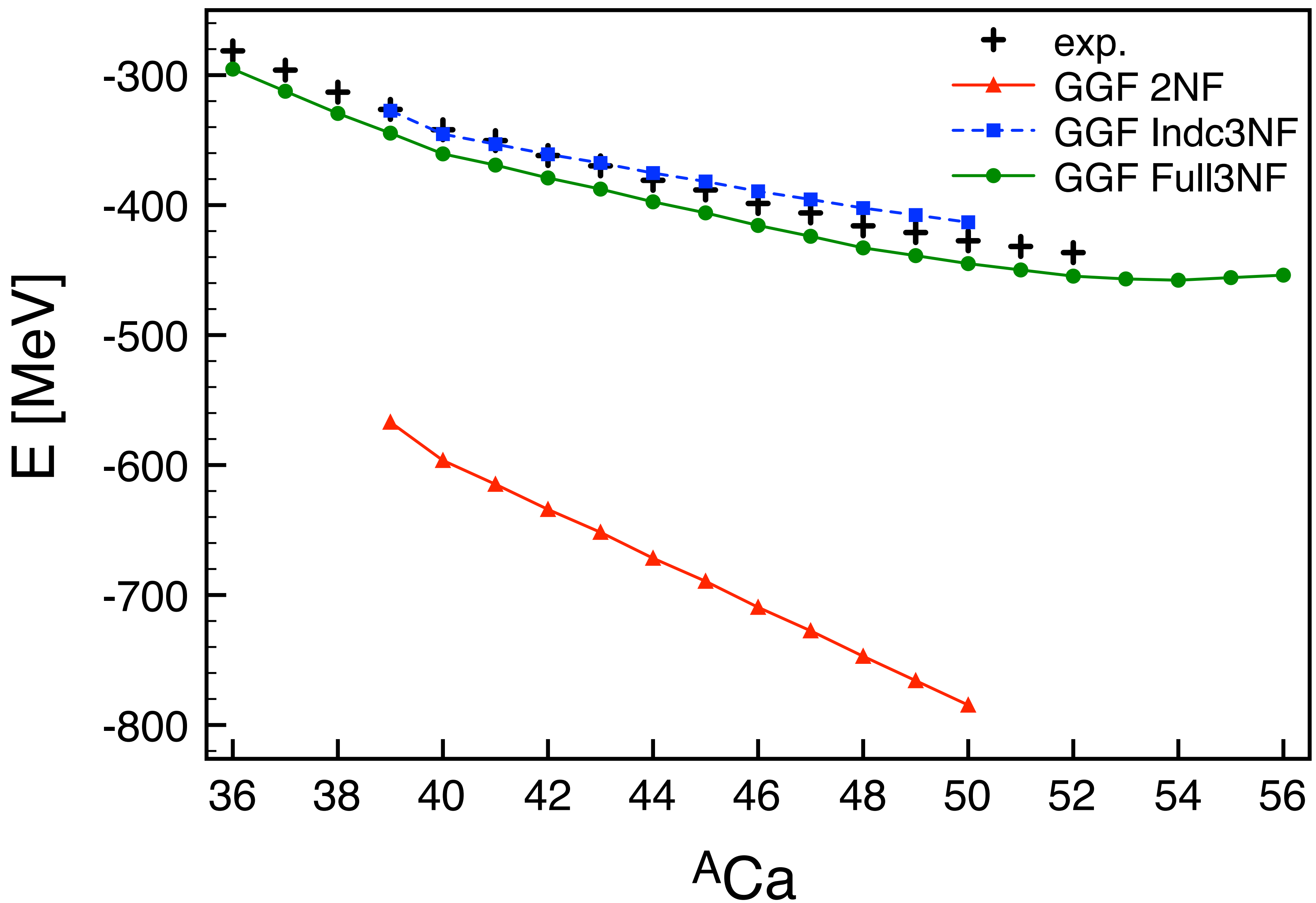
- 3N interaction: chiral N²LO (400 MeV) SRG-evolved to 2.0 fm⁻¹ [Navrátil 2007]

  ➟ Fit to three- and four-body systems only

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

Calcium isotopic chain

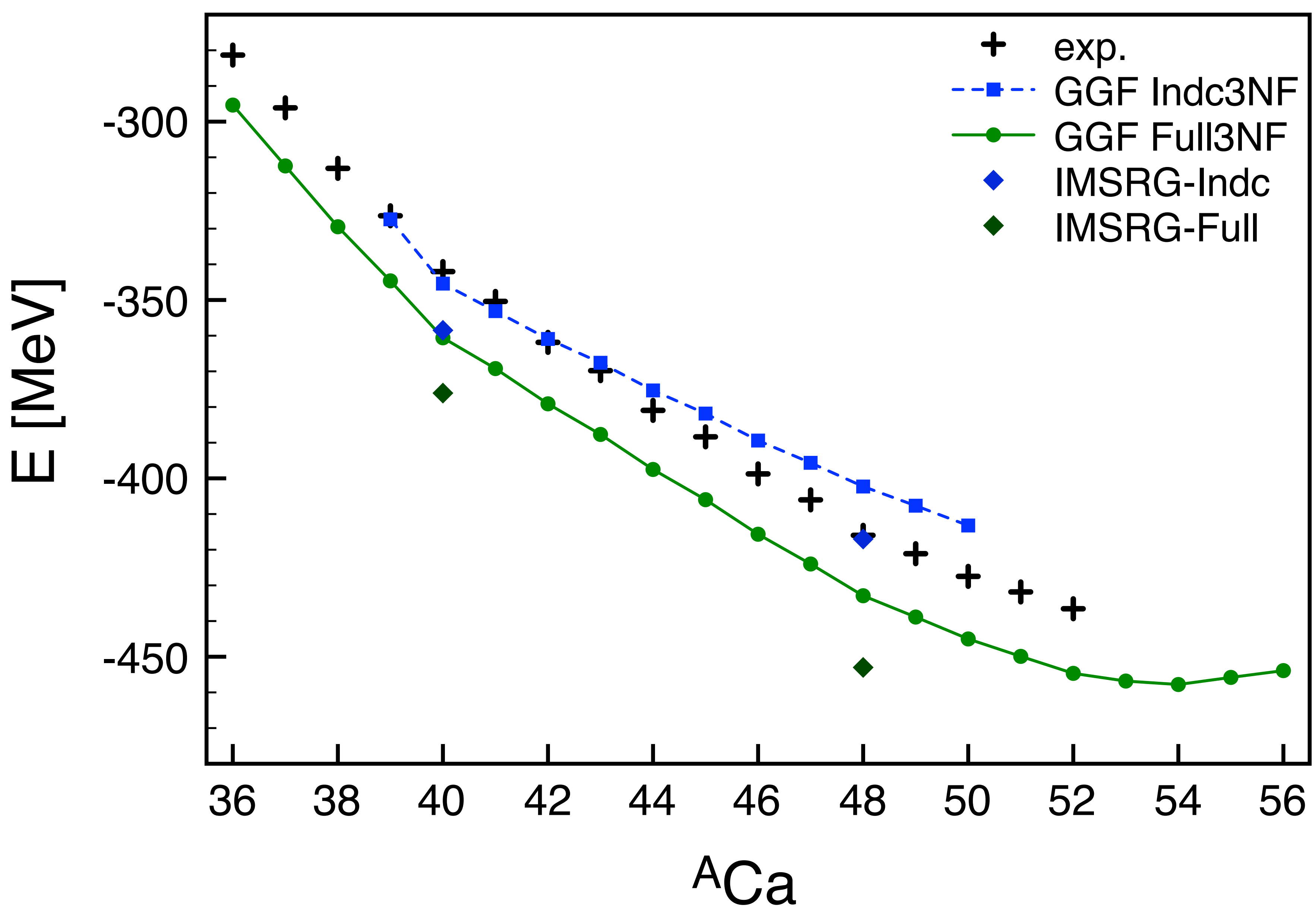
- First *ab initio* calculation of the whole Ca chain with NN + 3N forces
  - ➟ 3NF bring energies close to experiment
  - ➟ Induced 3NF and full 3NF investigated



Calcium isotopic chain

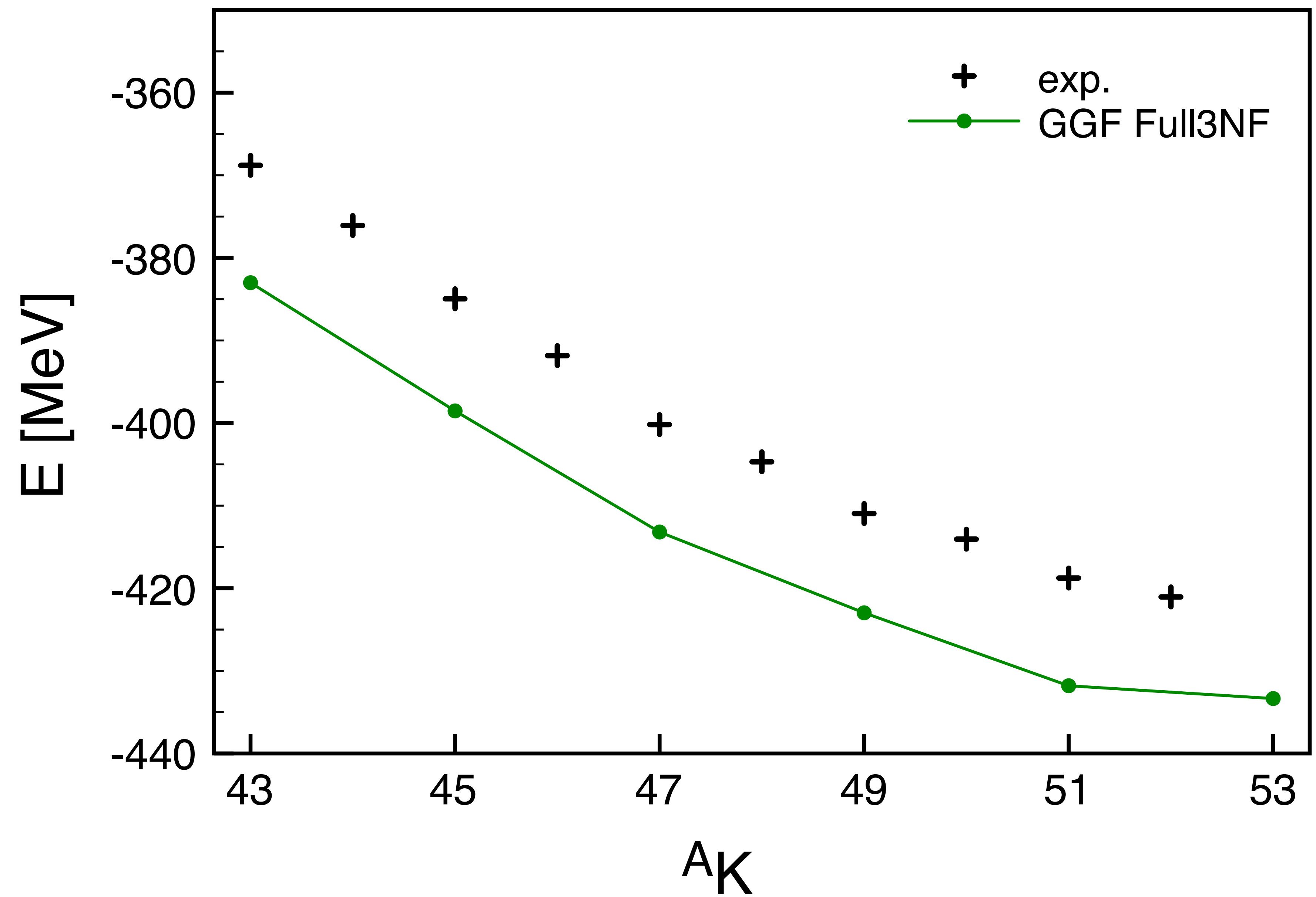
➟ Original 3NF correct the energy curvature

➟ Good agreement with IM-SRG (quantitative when 3rd order included)



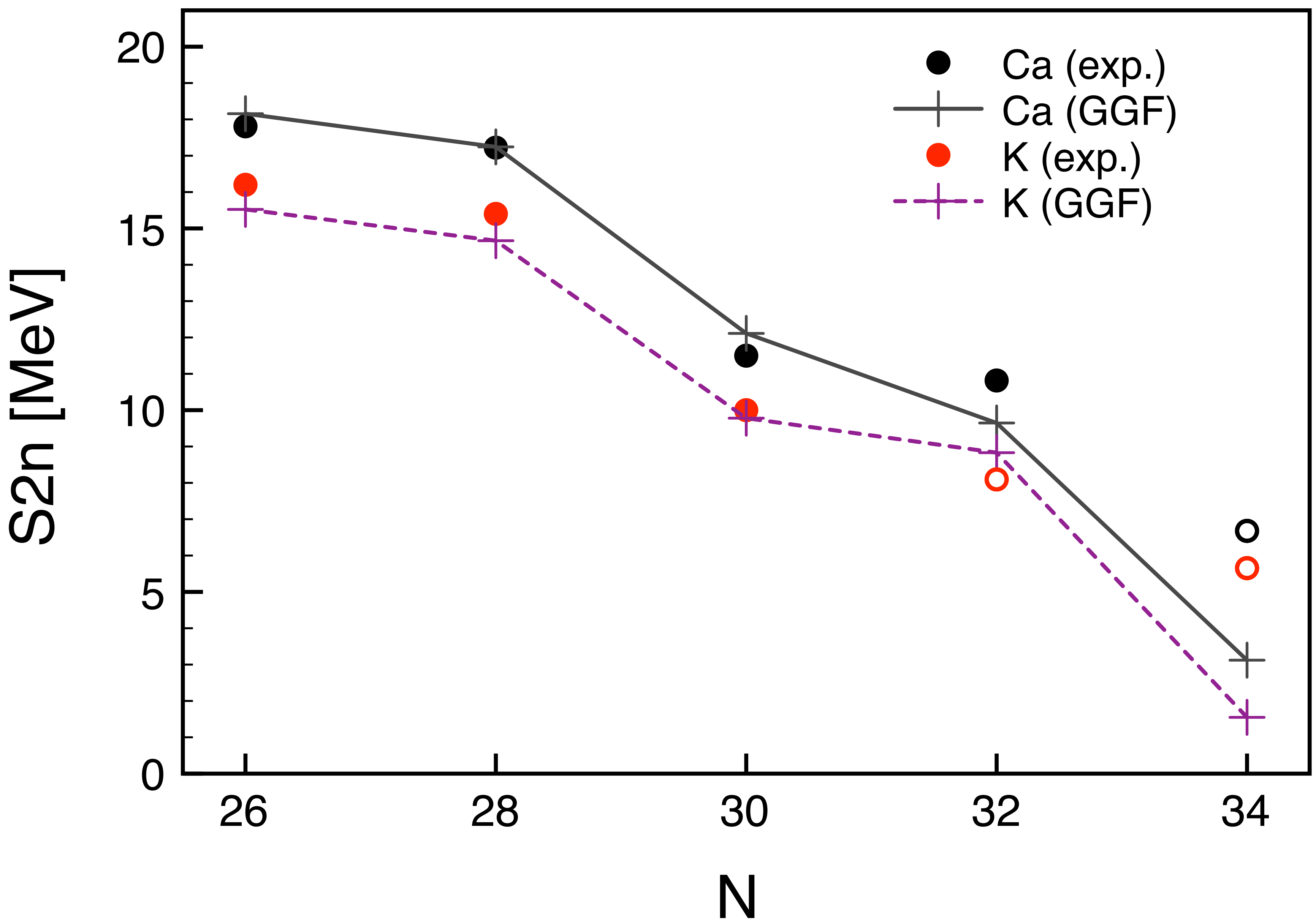
Potassium isotopic chain

- 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

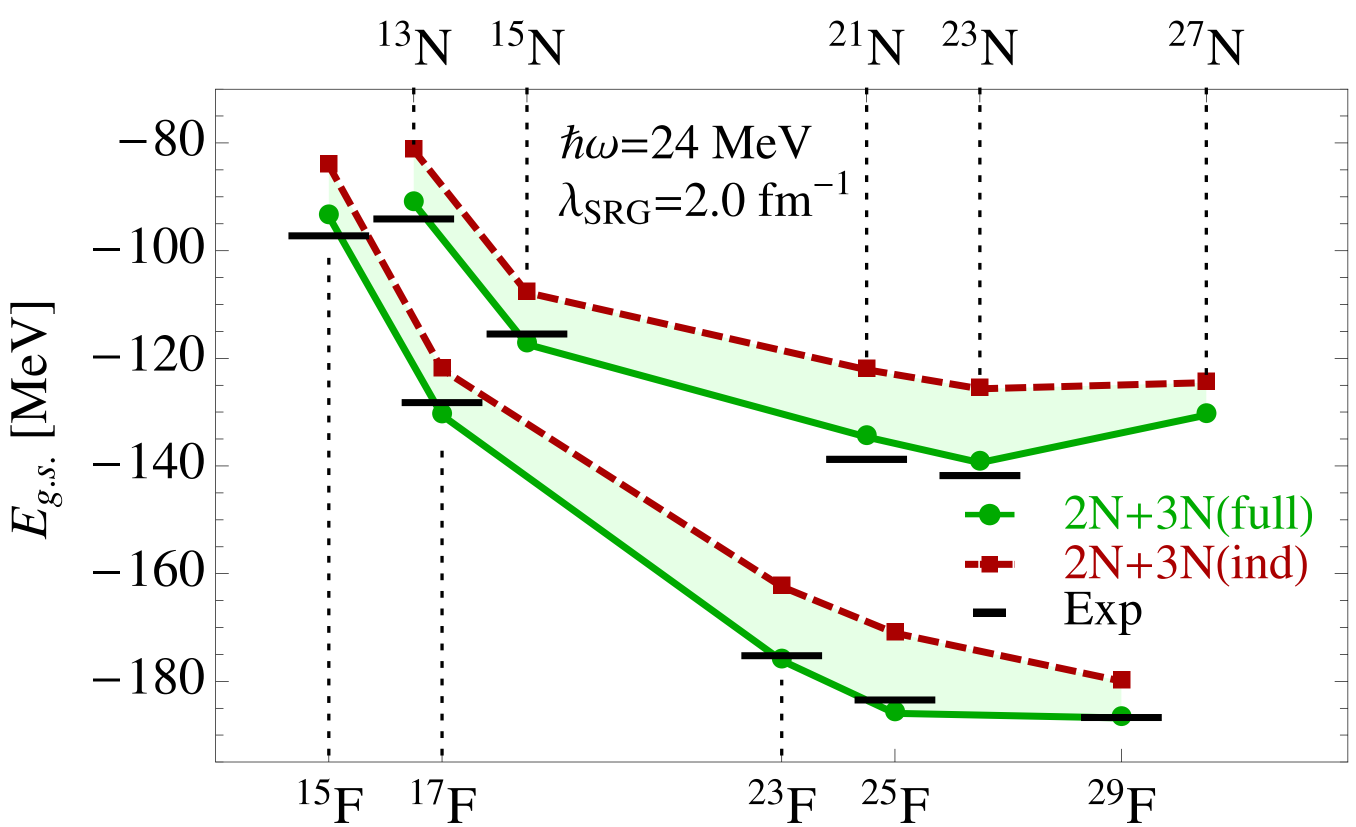


Benchmarks and chiral EFT interactions

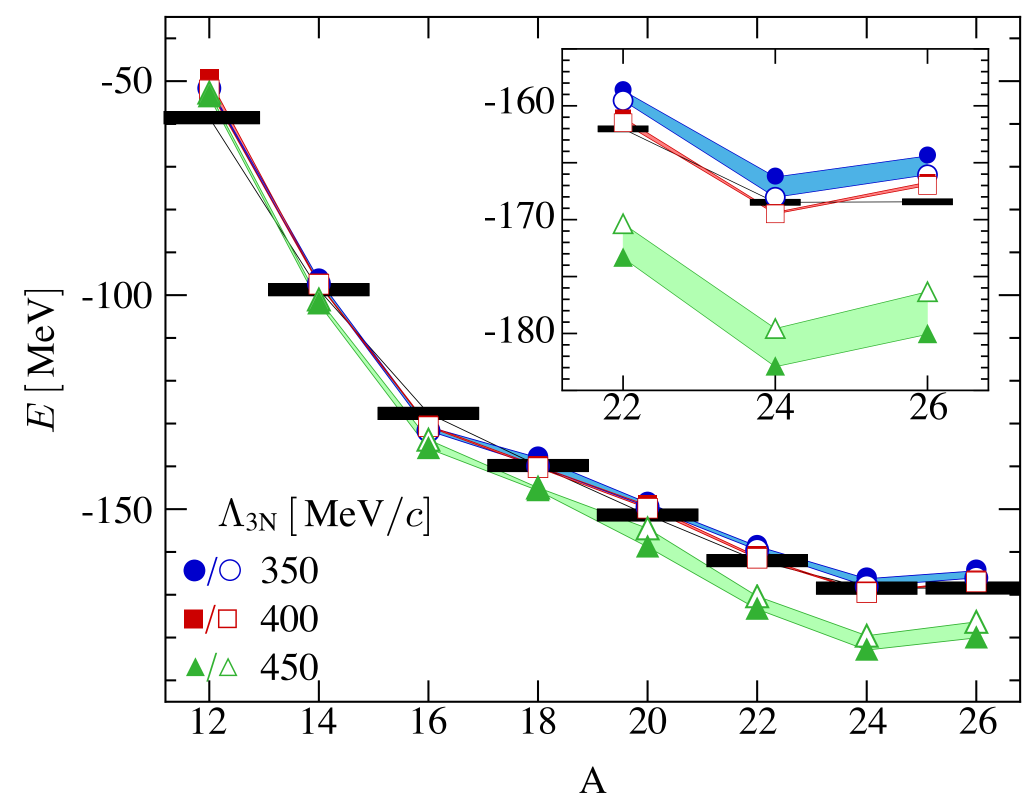
- *Ab initio* calculations as a test for chiral EFT interactions

- 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]

Spectrum and spectroscopic factors

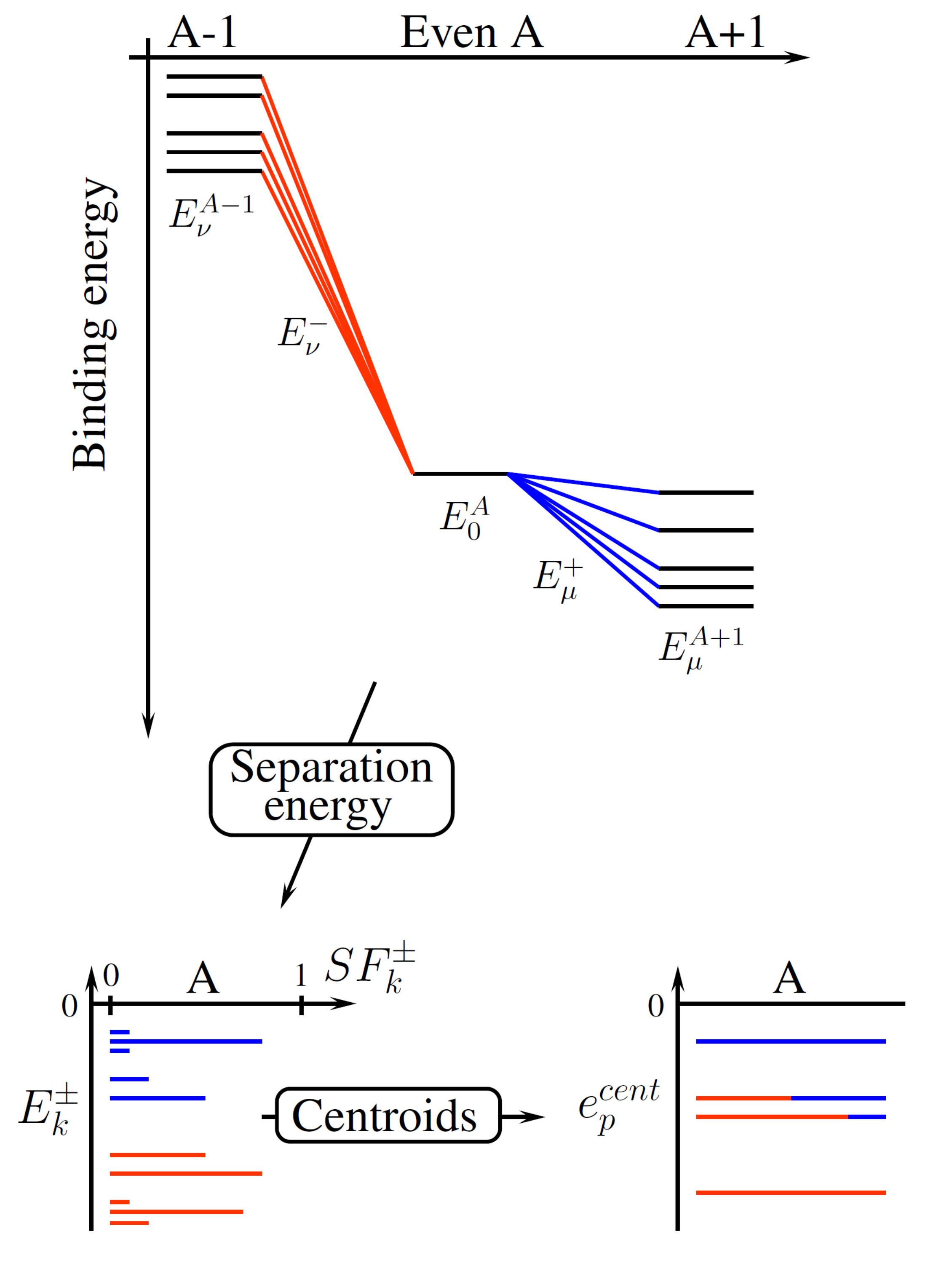
✺ Separation energy spectrum

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

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



[figure from Sadoudi]

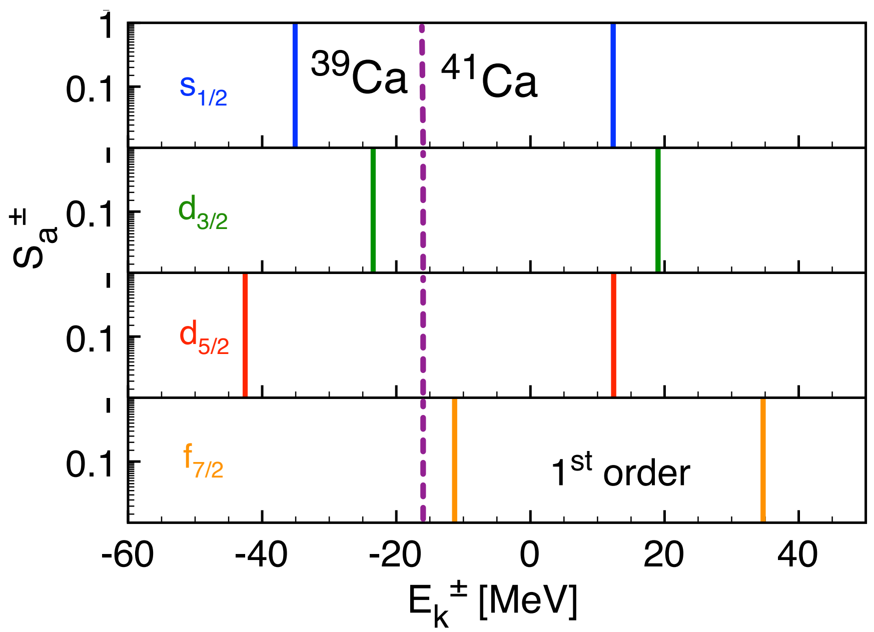
✺ Spectroscopic factors

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

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

Spectral strength distribution

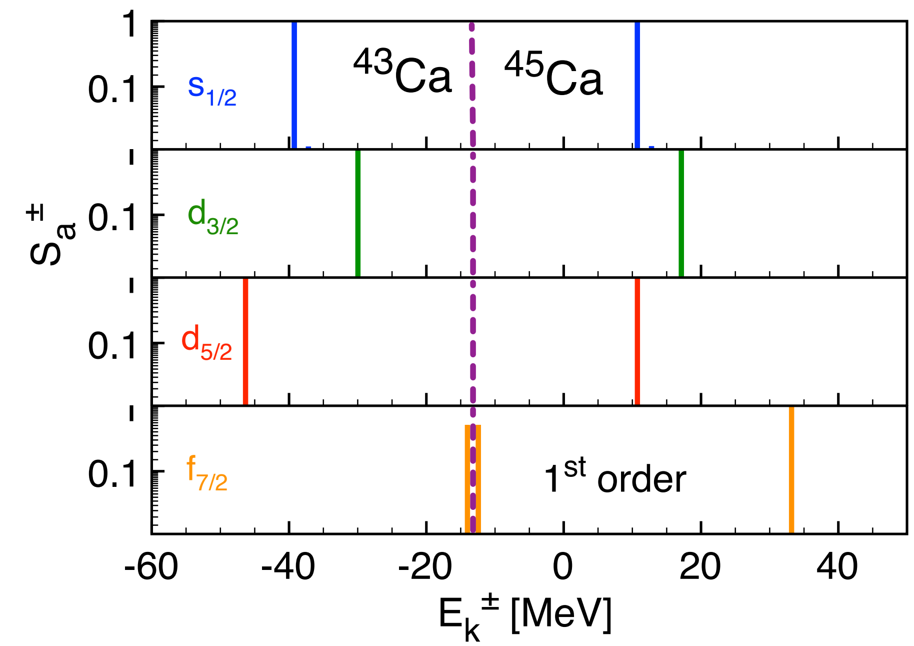
Dyson 1st order (HF)



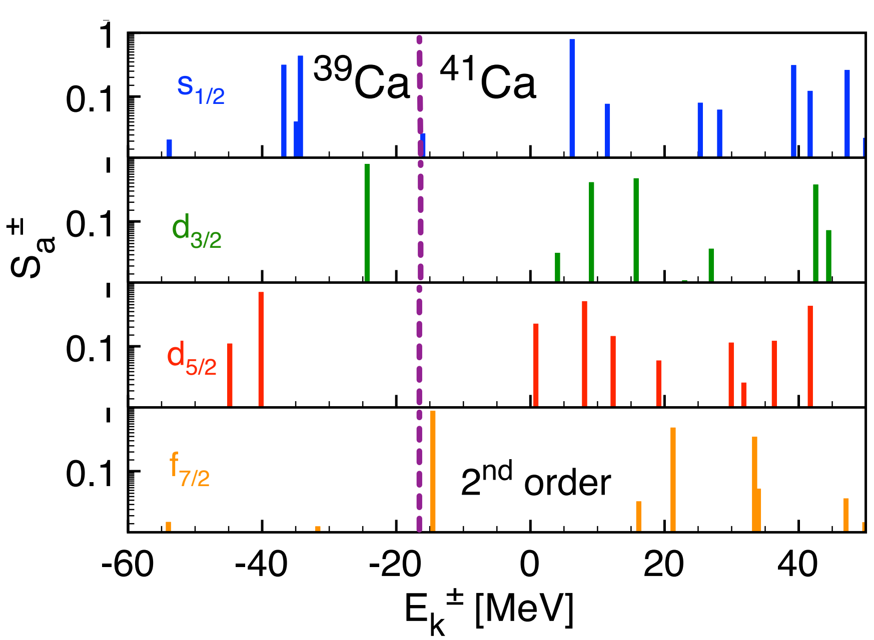
Fragmentation

Static pairing →

Gorkov 1st order (HFB)

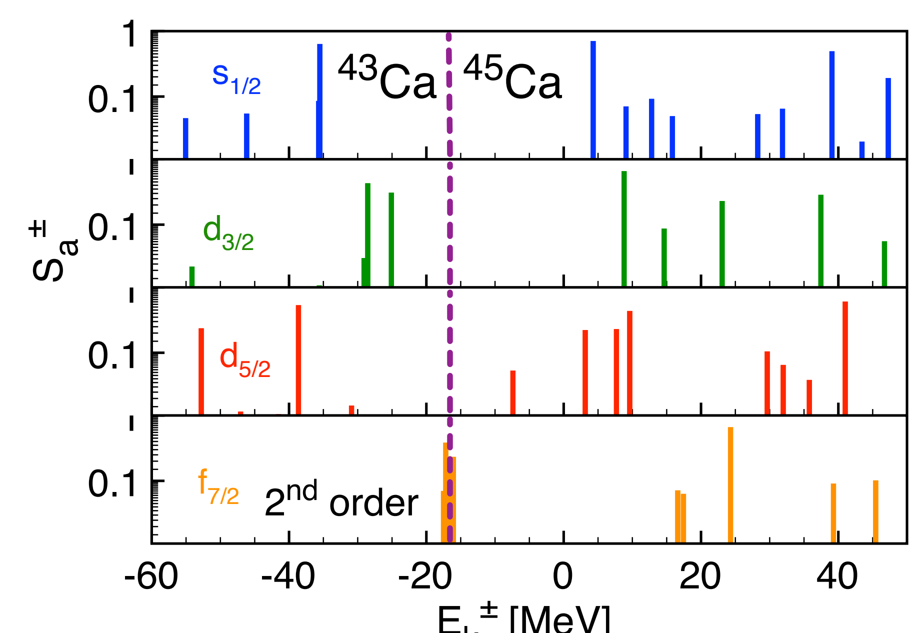


Dyson 2nd order



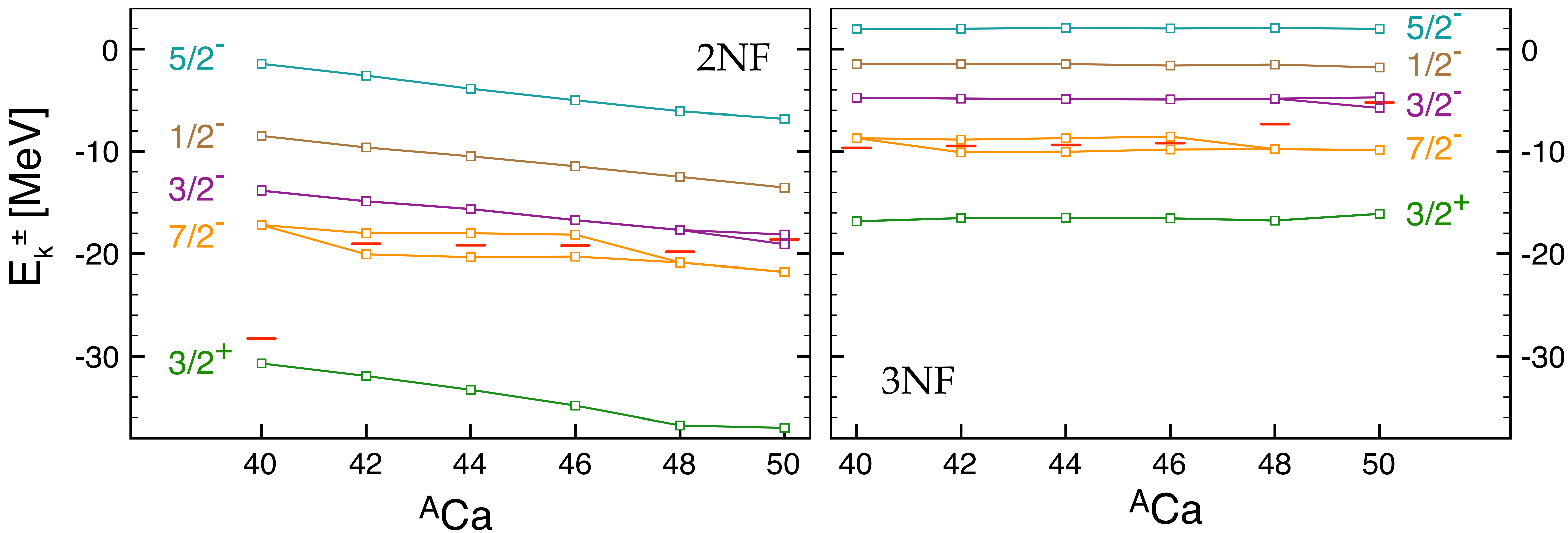
Dynamical fluctuations ↓

Gorkov 2nd order



Shell structure evolution

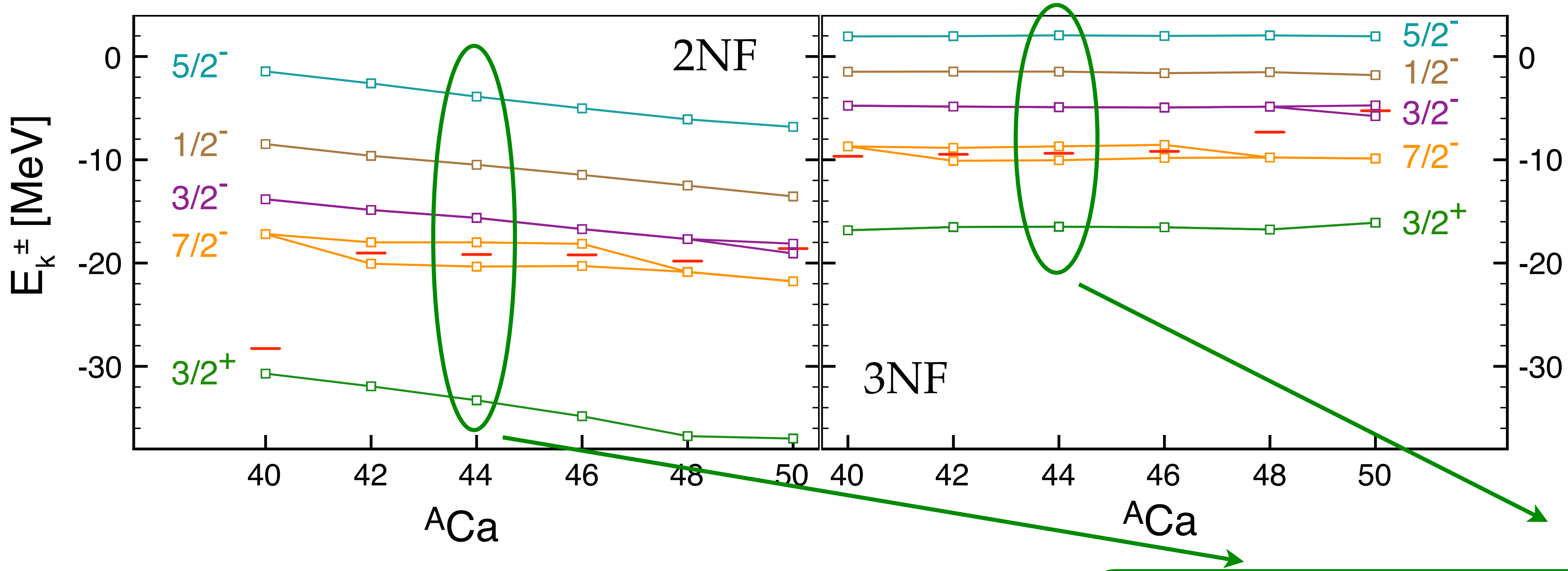
- One-neutron separation energies



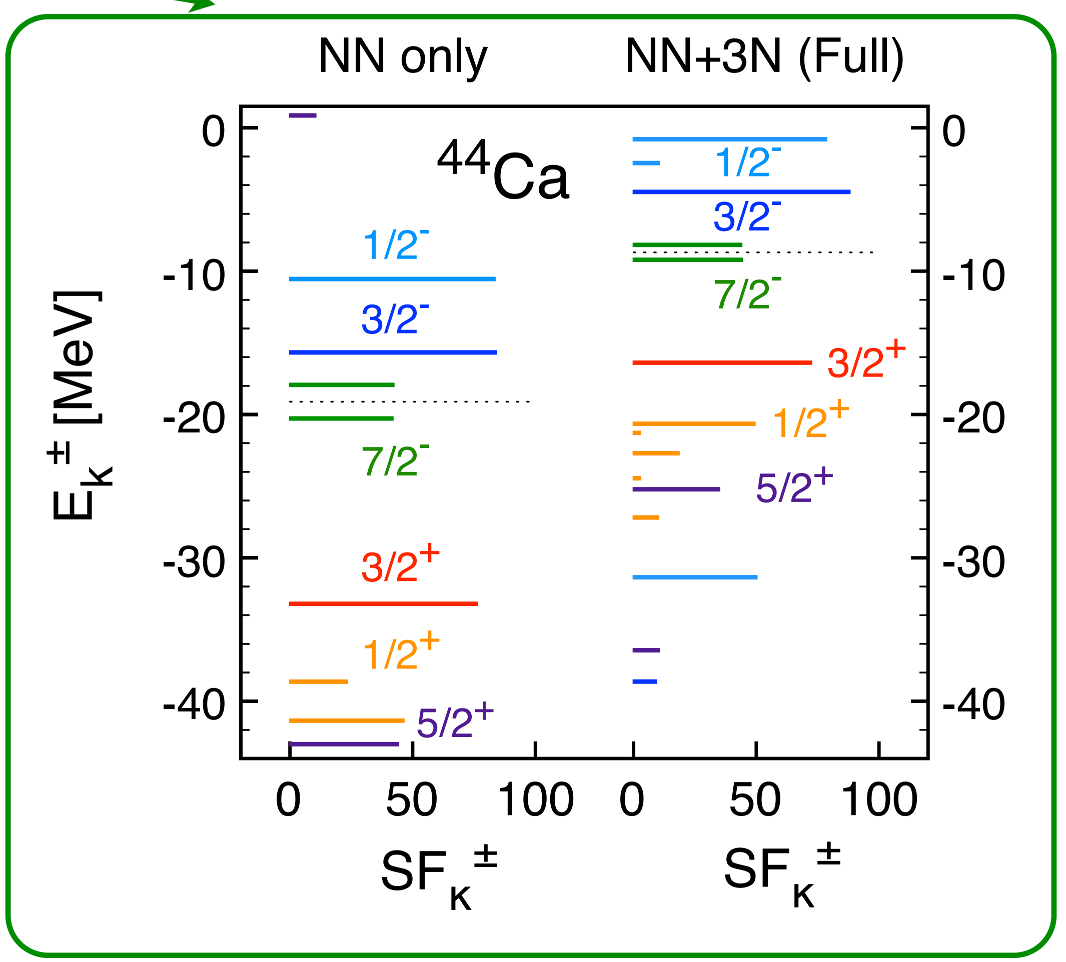
➟ Static and dynamic pairing correlations

➟ 3NF significantly compress spectrum

Shell structure evolution



* NN vs. NN+3NF in ^{44}Ca
  * ➟ Similar degree of fragmentation
  * ➟ SF of main peaks not much affected



Shell structure evolution

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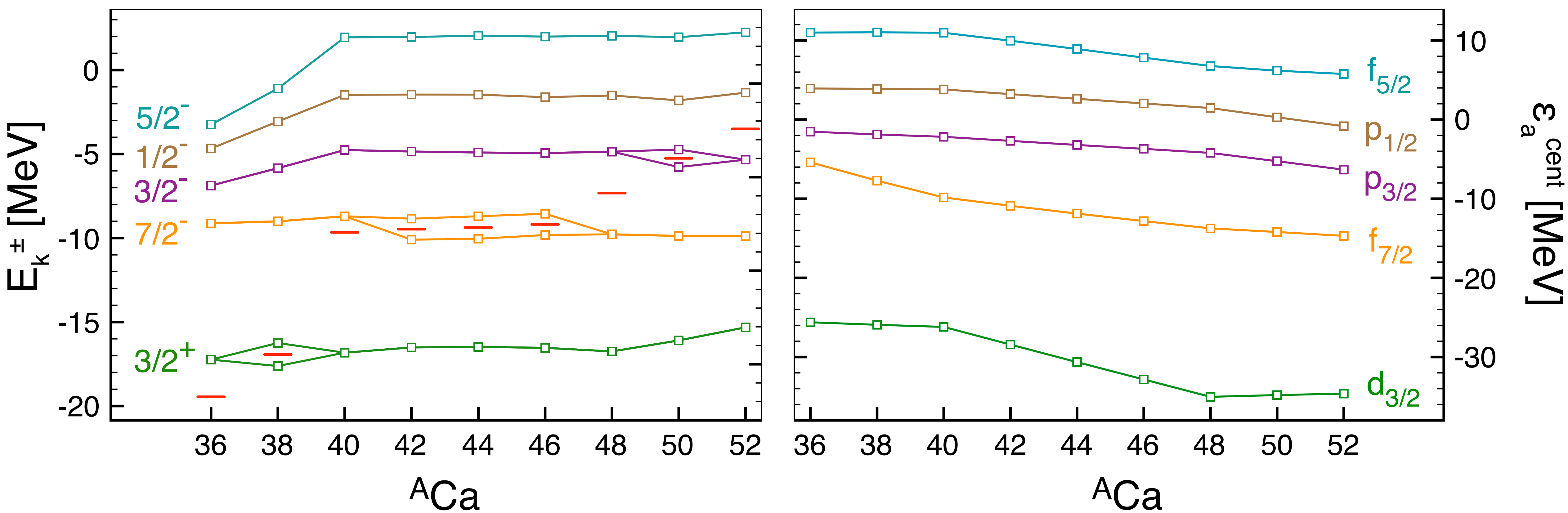
✺ ESPE collect fragmentation of "single-particle" strengths from both N±1

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

[Baranger 1970, Duguet and Hagen 2011]

Separation energies

Centroids



Conclusions and outlook (part II)

✺ Gorkov-Green's functions:

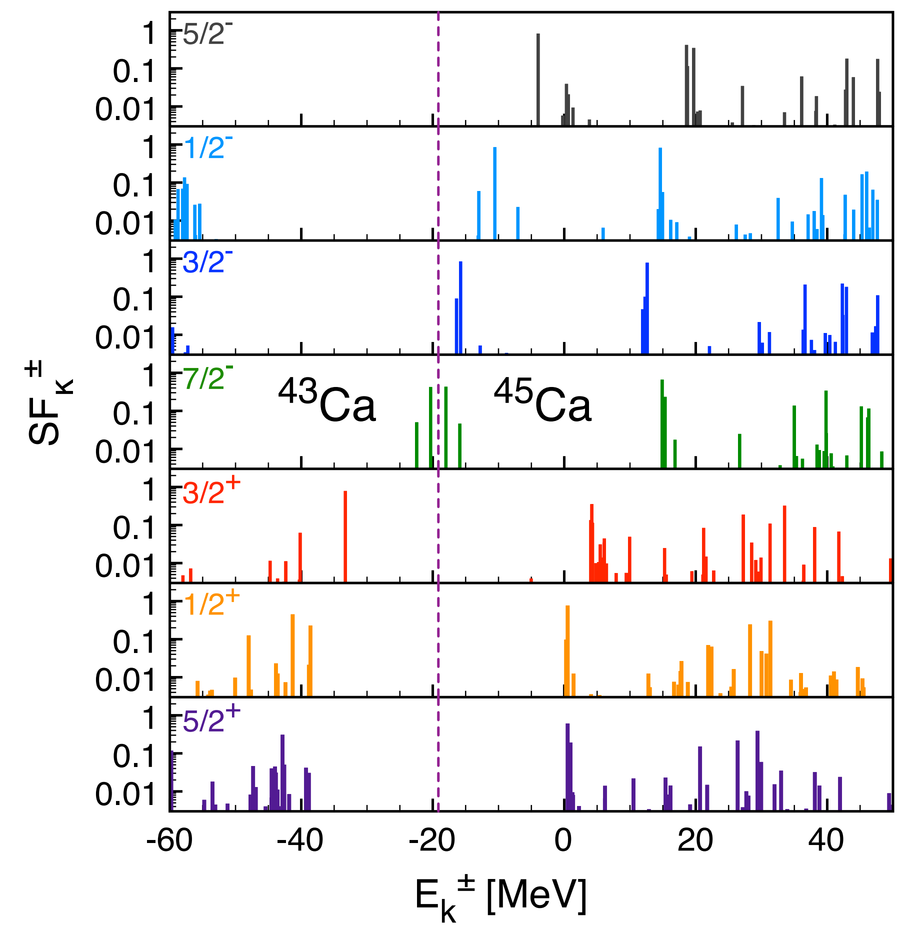
➟ Manageable route to (near) degenerate systems

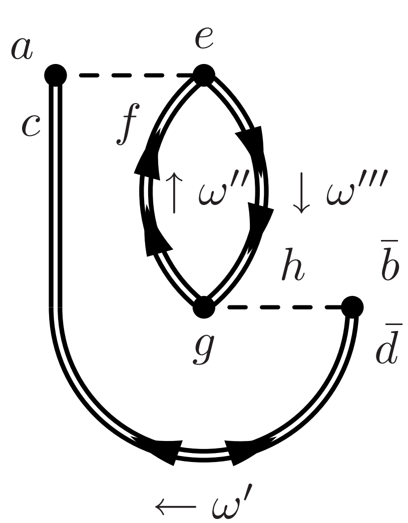
➟ First *ab initio* description of medium-mass chains

➟ 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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