Gorkov-Green's functions in mid-mass nuclei with chiral interactions

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with

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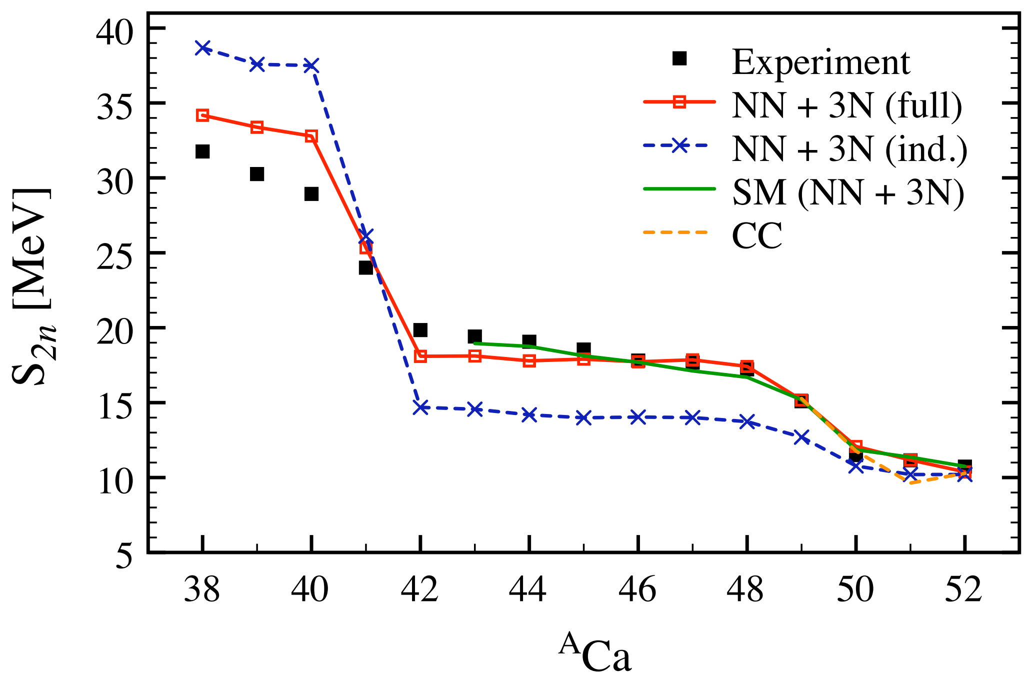

Nuclear structure & reactions: experimental and ab initio theoretical perspectives

TRIUMF, 21 February 2014

Going *open-shell:* Gorkov-Green's functions

- ✪ Self-consistent Green's functions
  - ➟ Many-body truncation in the self-energy expansion (cf. CC, IM-SRG, ...)
  - ➟ Access to *A±1* systems via spectral function
  - ➟ Natural connection to scattering (e.g. optical potentials)

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- Formulate the expansion scheme around a Bogoliubov vacuum
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- *Formalism* VS, Duguet & Barbieri, PRC 84 064317 (2011)
- *Proof of principle* VS, Barbieri & Duguet, PRC 87 011303 (2013)
- *Technical aspects* VS, Barbieri & Duguet, arXiv:1311.1989 (2013)
- *NN+3N* VS, Cipollone, Barbieri, Navrátil & Duguet, arXiv:1312.2068 (2013)

Gorkov 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 $\Omega = H - \mu A$

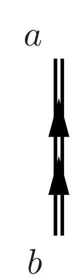
➟ $|\Psi_0\rangle$ minimizes $\Omega_0 = \langle \Psi_0 | \Omega | \Psi_0 \rangle$ under the constraint $A = \langle \Psi_0 | A | \Psi_0 \rangle$

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

✪ Set of 4 propagators

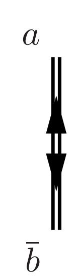
[Gorkov 1958]

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



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

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



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

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

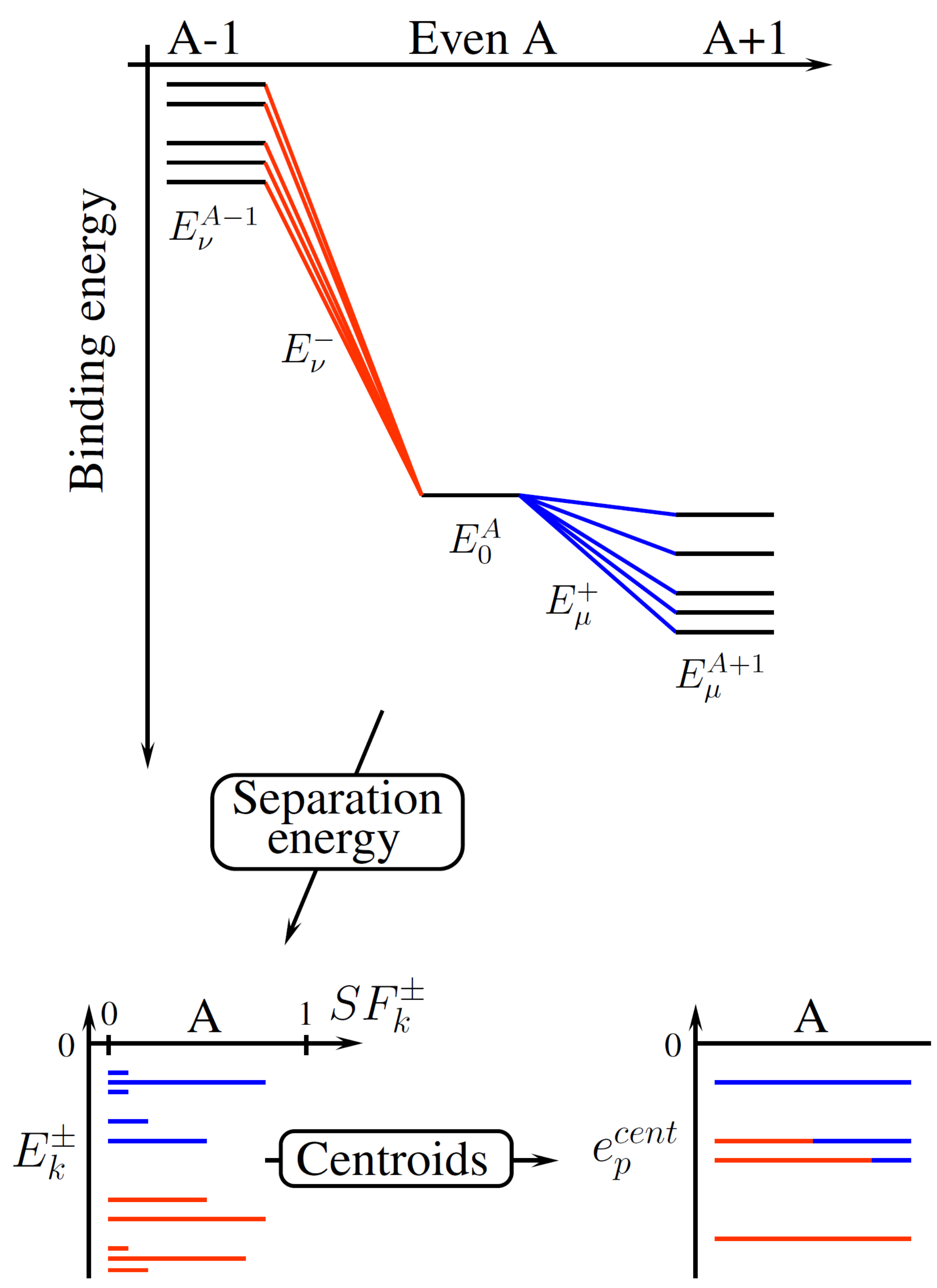
where
$$\begin{cases} \mathcal{U}^{k*}_a \equiv \langle \Psi_k | a^\dagger_a | \Psi_0 \rangle \\ \mathcal{V}^{k*}_a \equiv \langle \Psi_k | \bar{a}_a | \Psi_0 \rangle \end{cases}$$

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

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

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



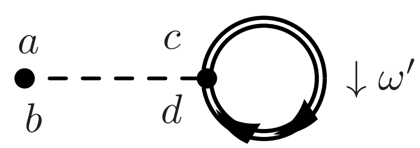
[figure from J. Sadoudi]

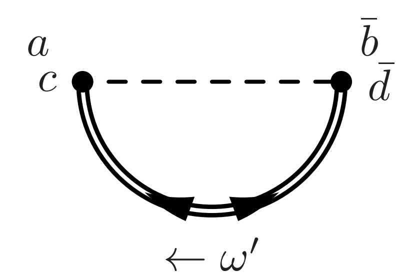
Gorkov equation

✪ Gorkov equation ⟶ energy *dependent* eigenvalue problem

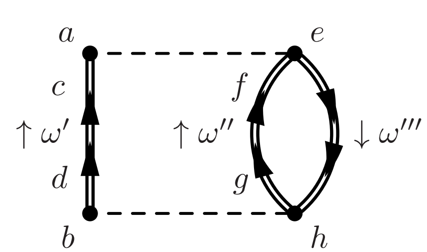
$$\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & -t_{ab} + \mu_{ab} + \Sigma^{22}_{ab}(\omega) \end{pmatrix}\Bigg|_{\omega_k} \begin{pmatrix} \mathcal{U}^k_b \\ \mathcal{V}^k_b \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k_a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

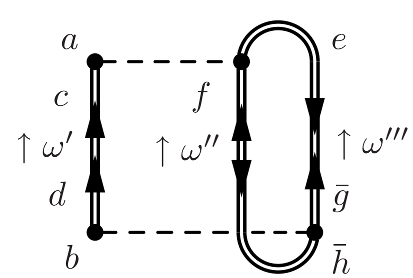
✪ 1st order ➟ energy-independent self-energy

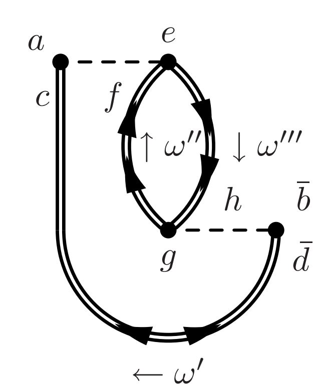
$\Sigma^{11\,(1)}_{ab} =$ 

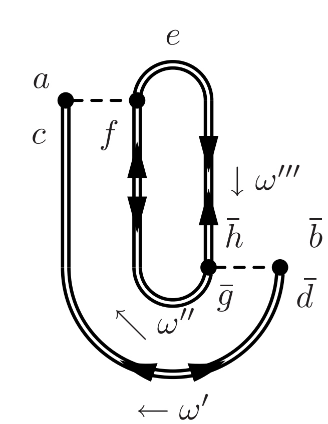
$\Sigma^{12\,(1)}_{ab} =$ 

✪ 2nd order ➟ energy-dependent self-energy

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

$+$ 

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

$+$ 

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[Schirmer & Angonoa 1989]

energy *independent* eigenvalue problem

$\propto N_b^3$

typically ~10^6-10^7

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

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Krylov space eigenvalue problem

$\propto N_{Lanczos}$

typically ~10^2-10^3

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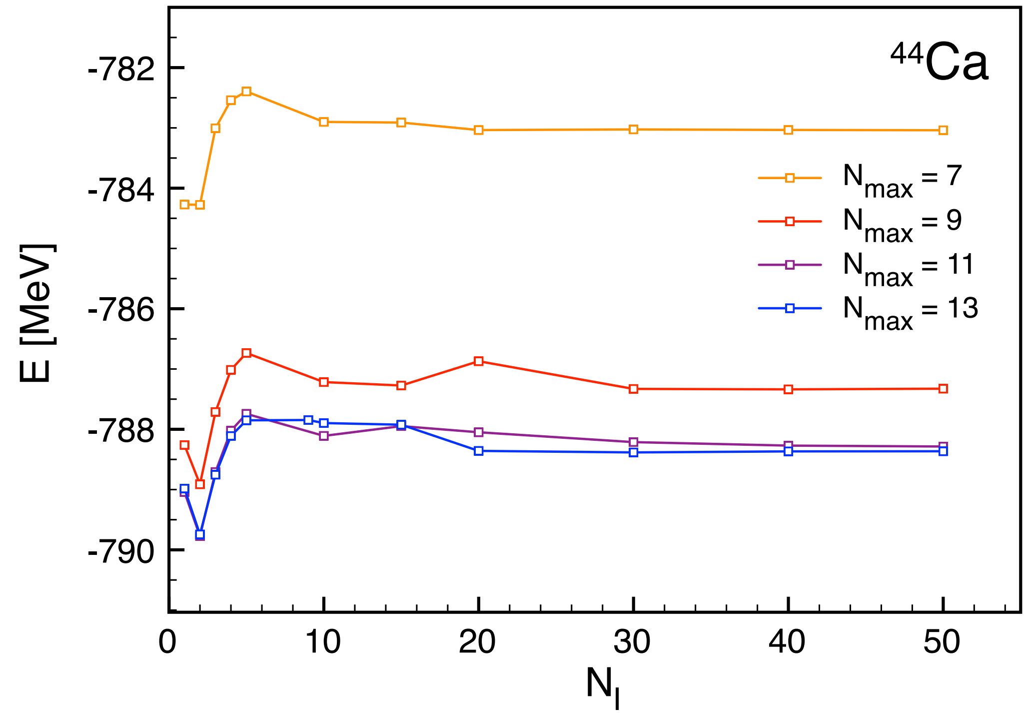
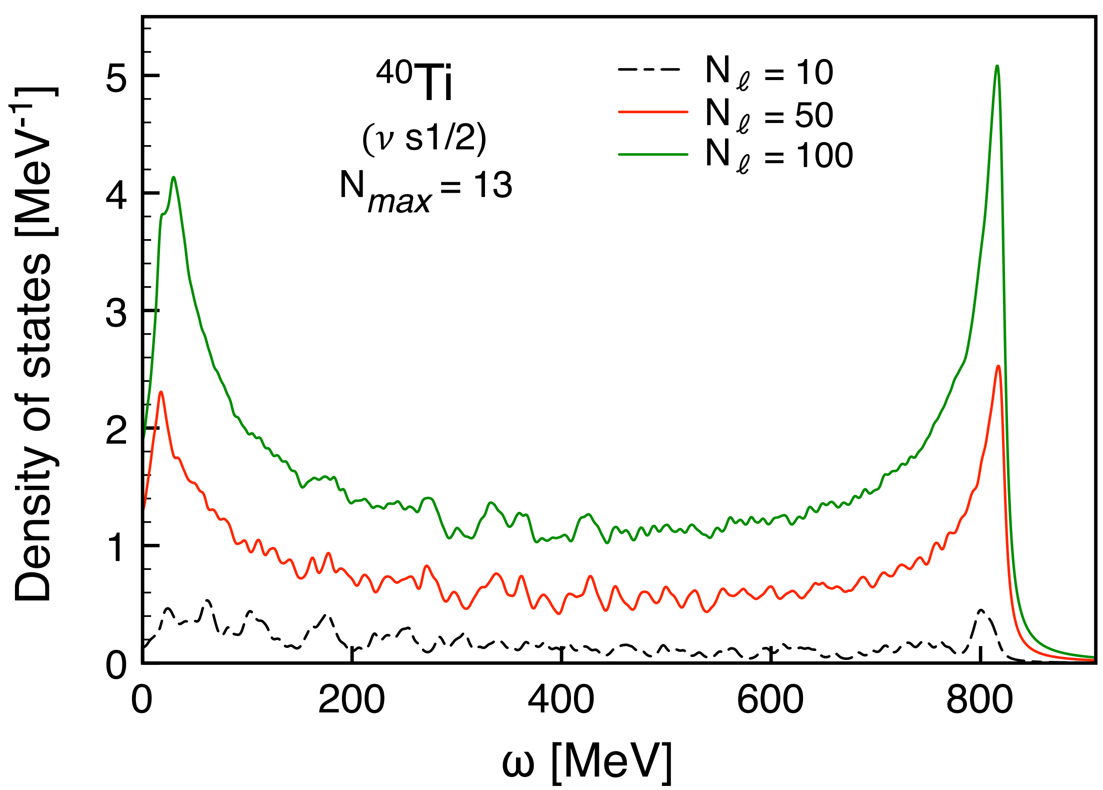
Testing Krylov projection

- ✪ Energy & spectral distribution independent of the projection
- ✪ Same behavior for all model spaces

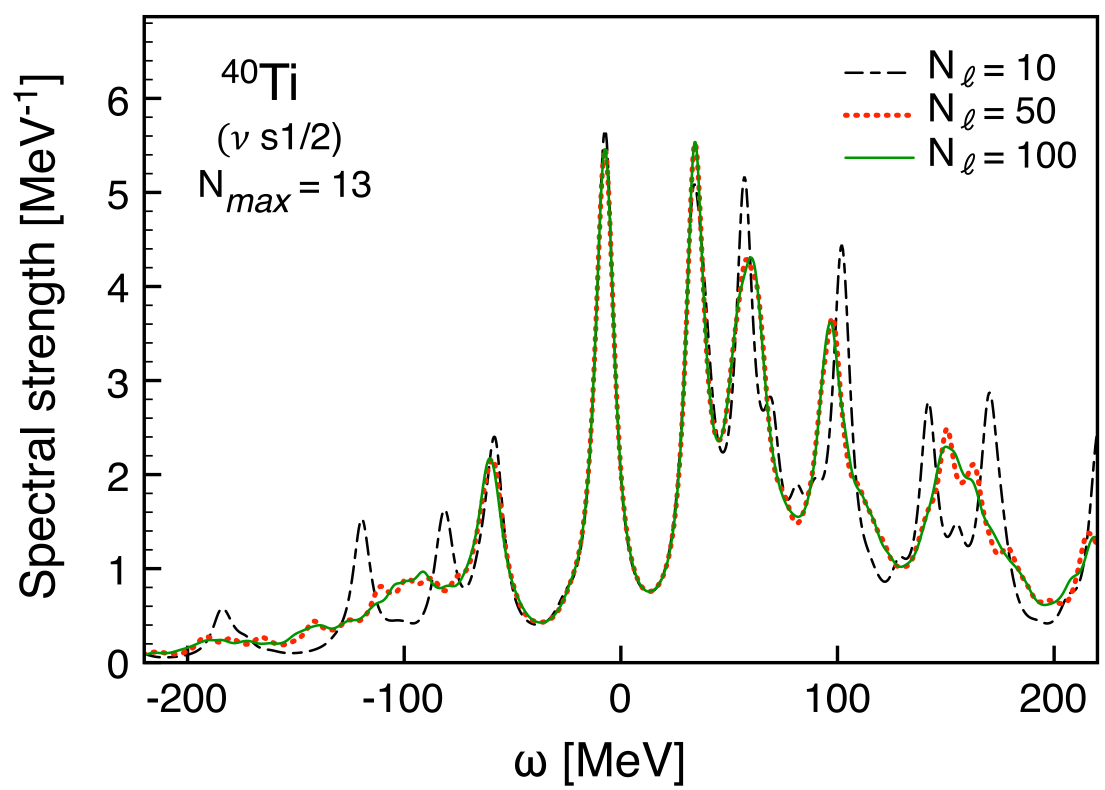
[VS, Barbieri & Duguet 2013]



Density of states



Spectral strength



Odd-even systems

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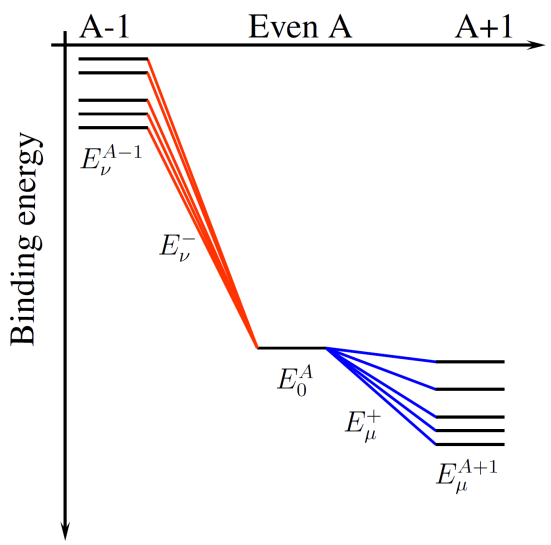
① From separation energies

➟ Either from A-1 or A+1



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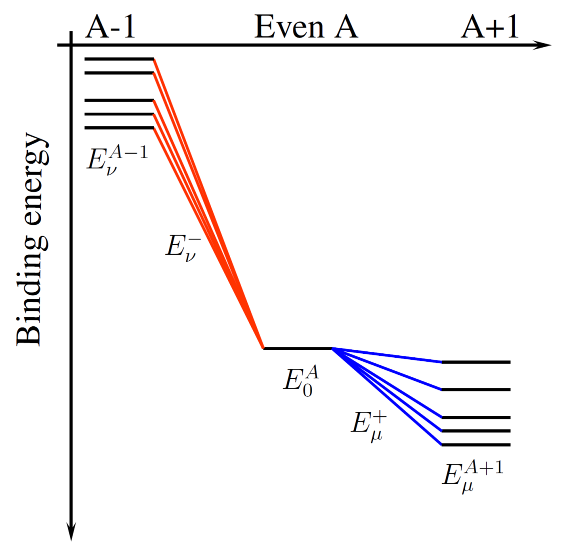

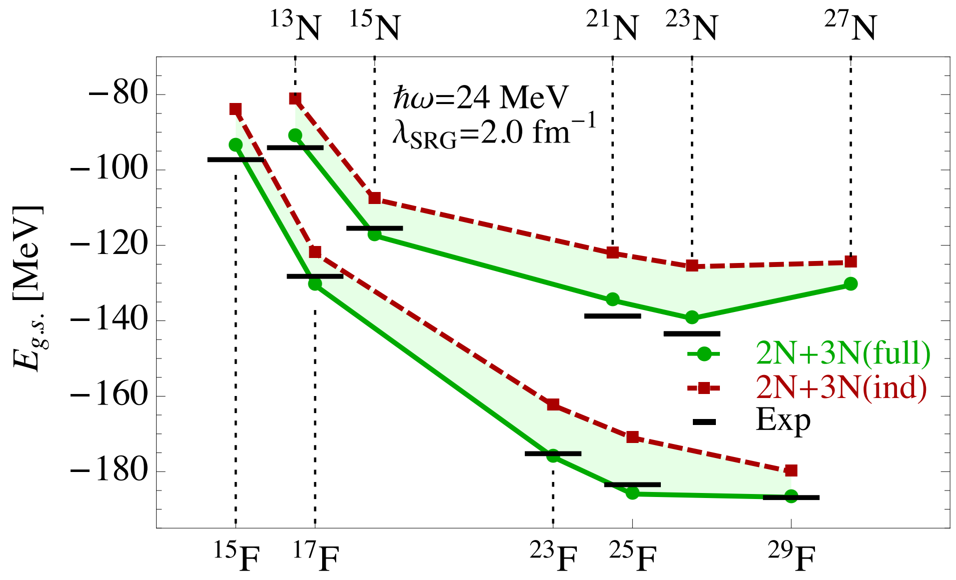

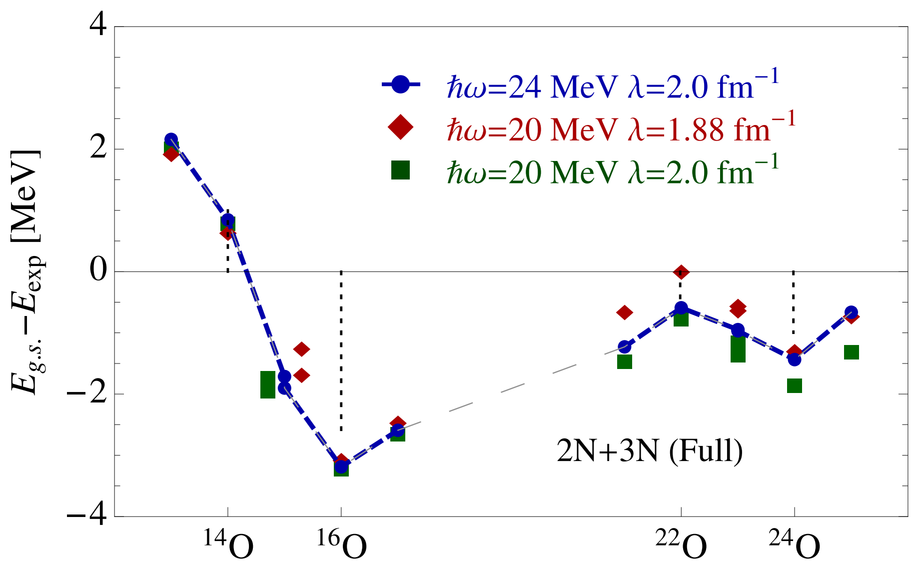

[Cipollone, Barbieri & Navrátil 2013]

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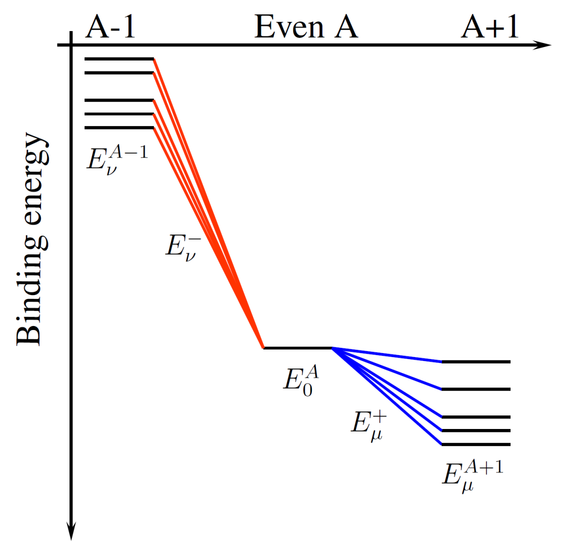
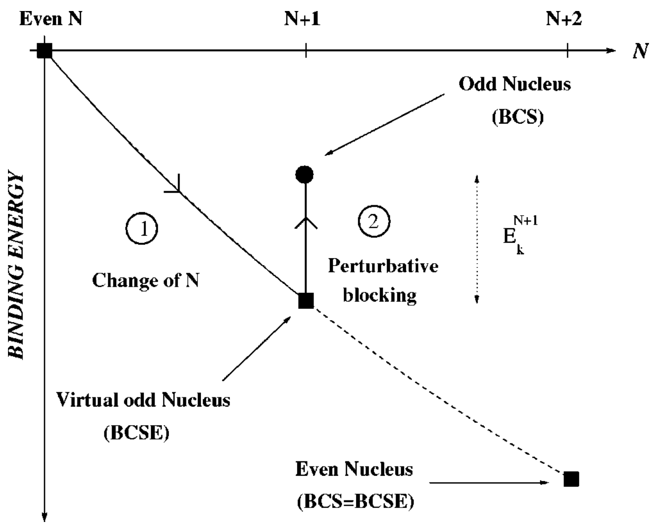


➟ "Fake" odd-A plus correction



[Duguet *et al.* 2001]

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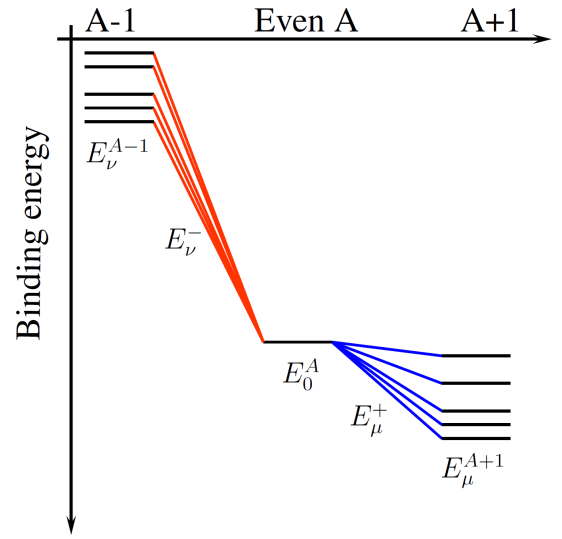

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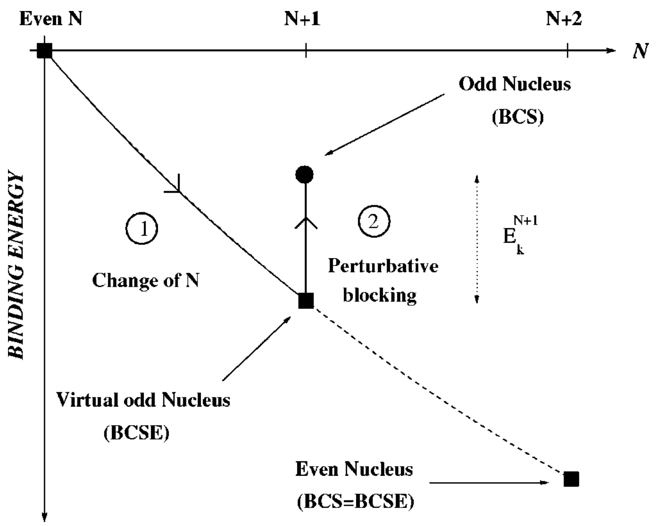


[Duguet *et al.* 2001]

Two methods agree within 2-300 keV

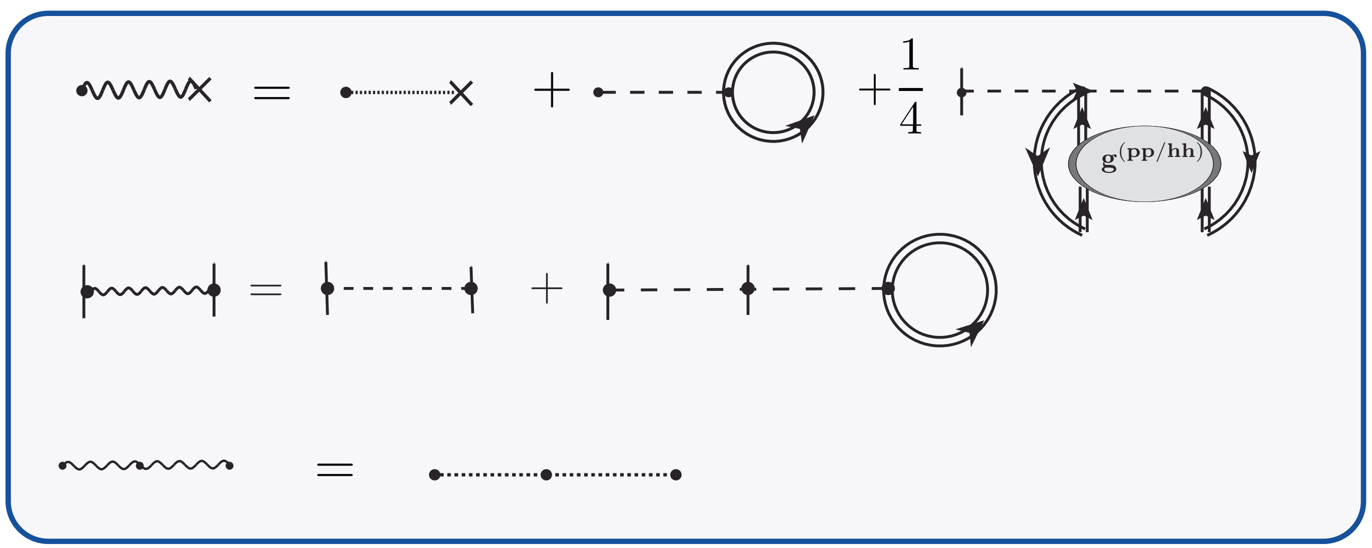
Three-body forces

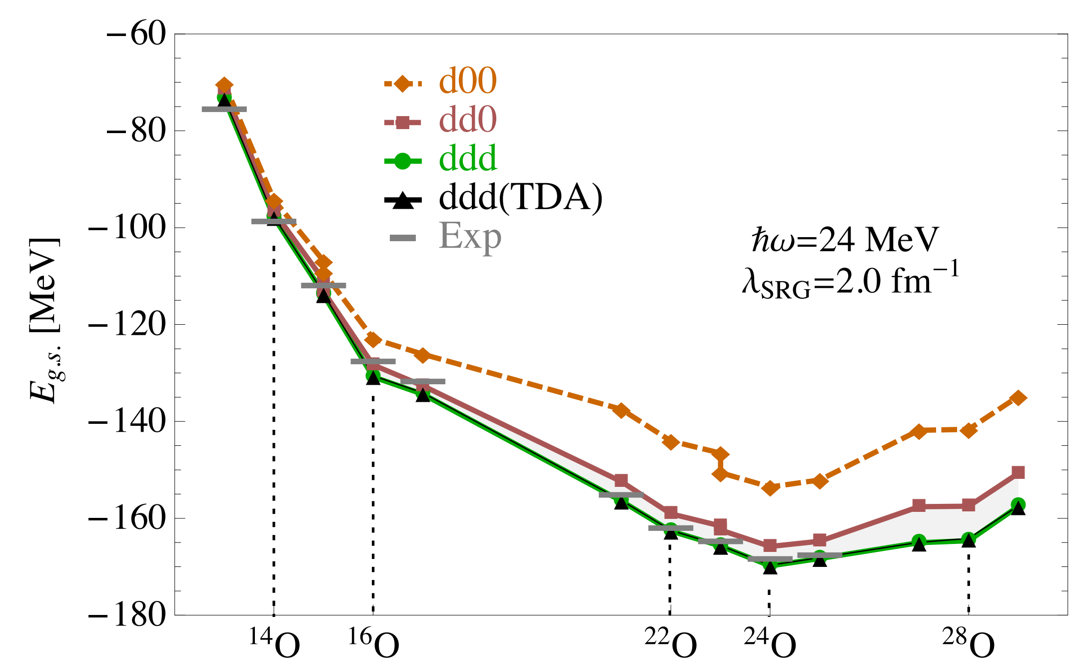
✪ One- and two-body forces derived from the 3N part of the Hamiltonian

➟ 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 significant extra correlations

The GGF input: NN & 3N interactions

✪ NN potential: chiral N^3LO (500 MeV) SRG-evolved to 2.0 fm^{-1}

[Entem and Machleidt 2003]

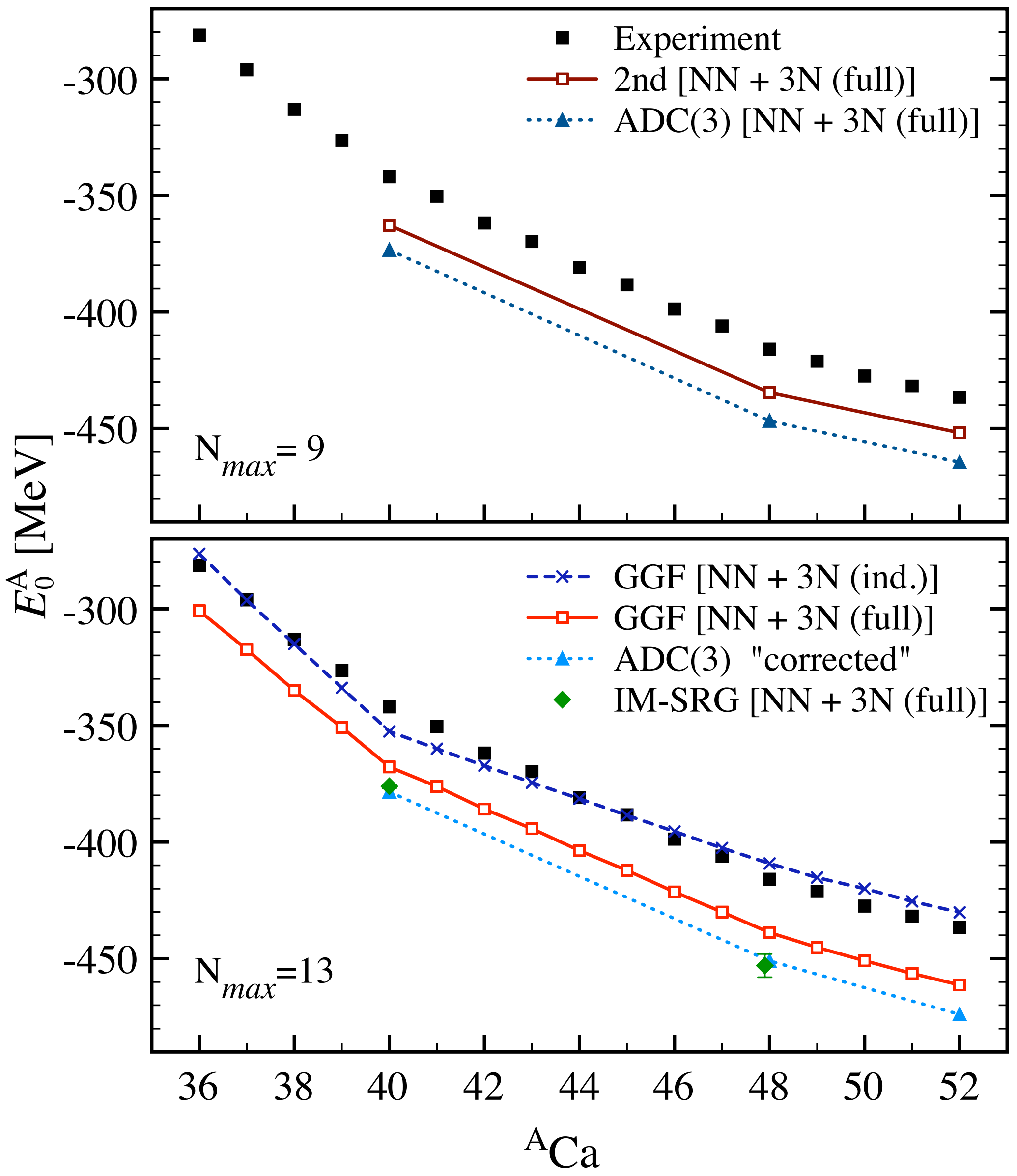
✪ 3N potential: chiral N^2LO (400 MeV) SRG-evolved to 2.0 fm^{-1} [Navrátil 2007]

- ➟ Fit to three- and four-body systems only
- ➟ Modified cutoff to reduce induced 4N contributions [Roth *et al*. 2012]

✪ In the future:

- ➟ Chiral 3NF at N^3LO
- ➟ Δ-full chiral interactions
- ➟ NN & 3N consistently SRG-evolved in momentum space
- ➟ ...
- ➟ Chiral interactions with improved/correct power counting
- ➟ Inputs from lattice QCD: couplings & YN interactions

Binding energies around Ca



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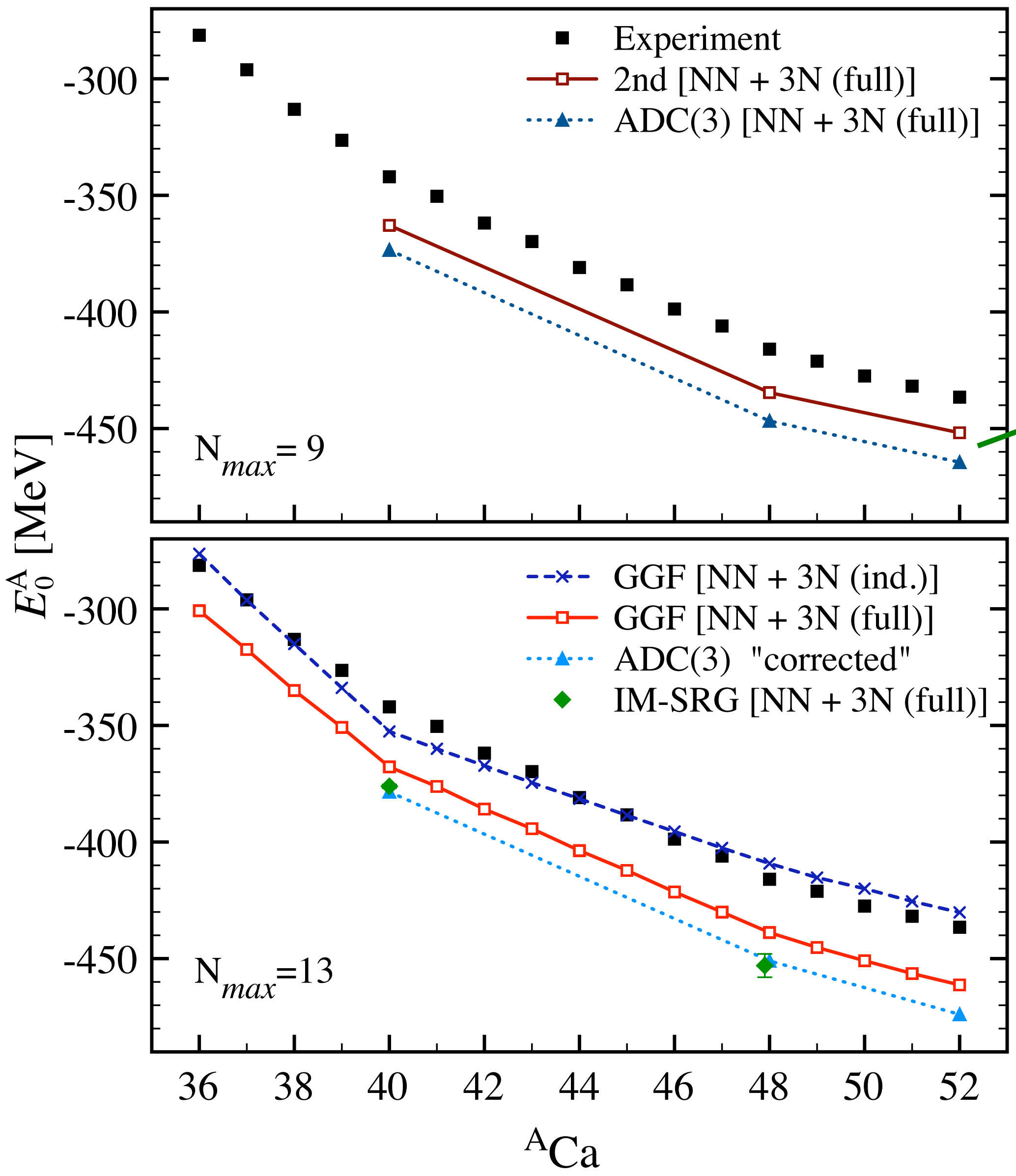

Estimate of the many-body truncation error

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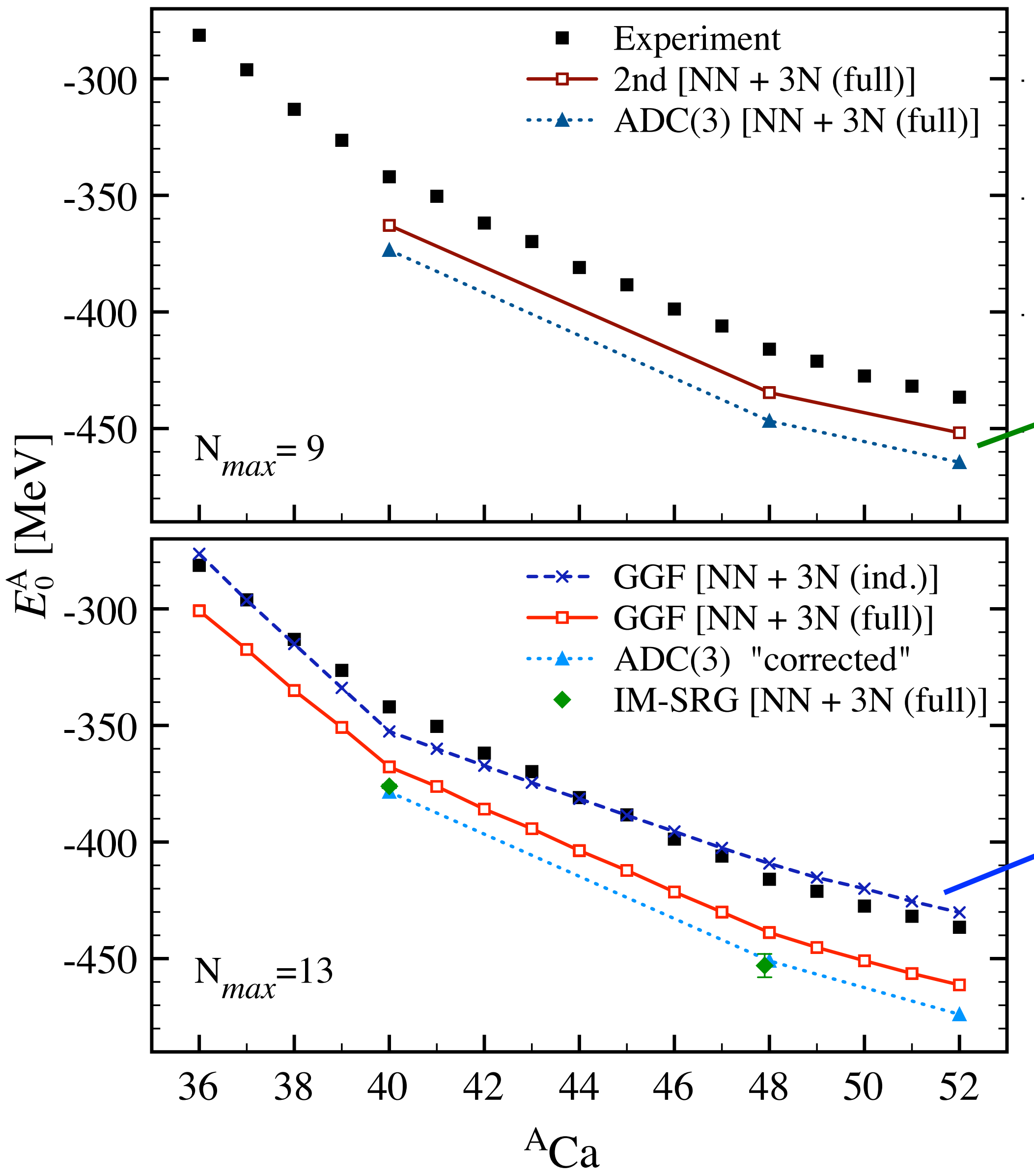

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Original 3NF correct for trend

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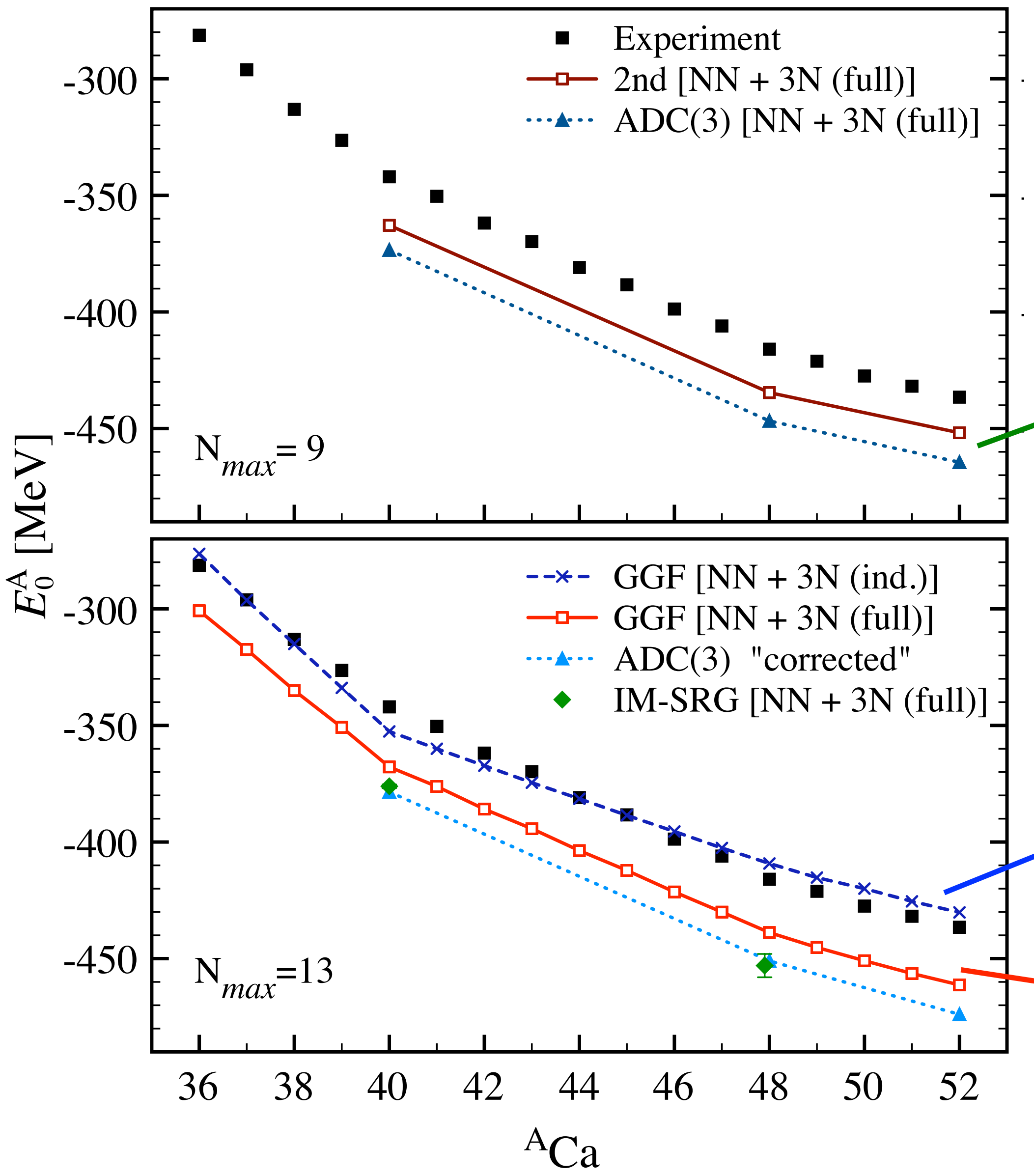

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Systematic overbinding

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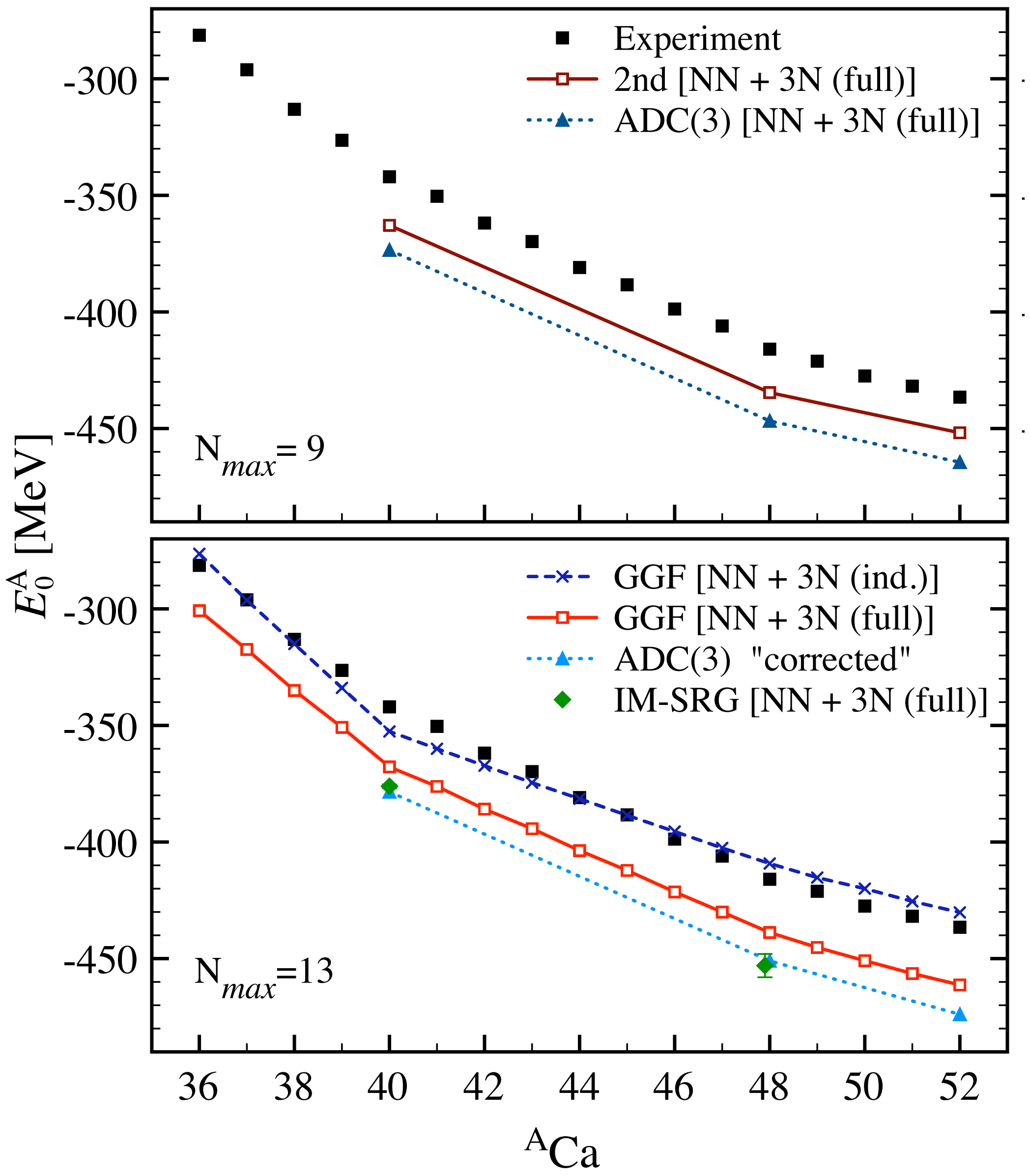
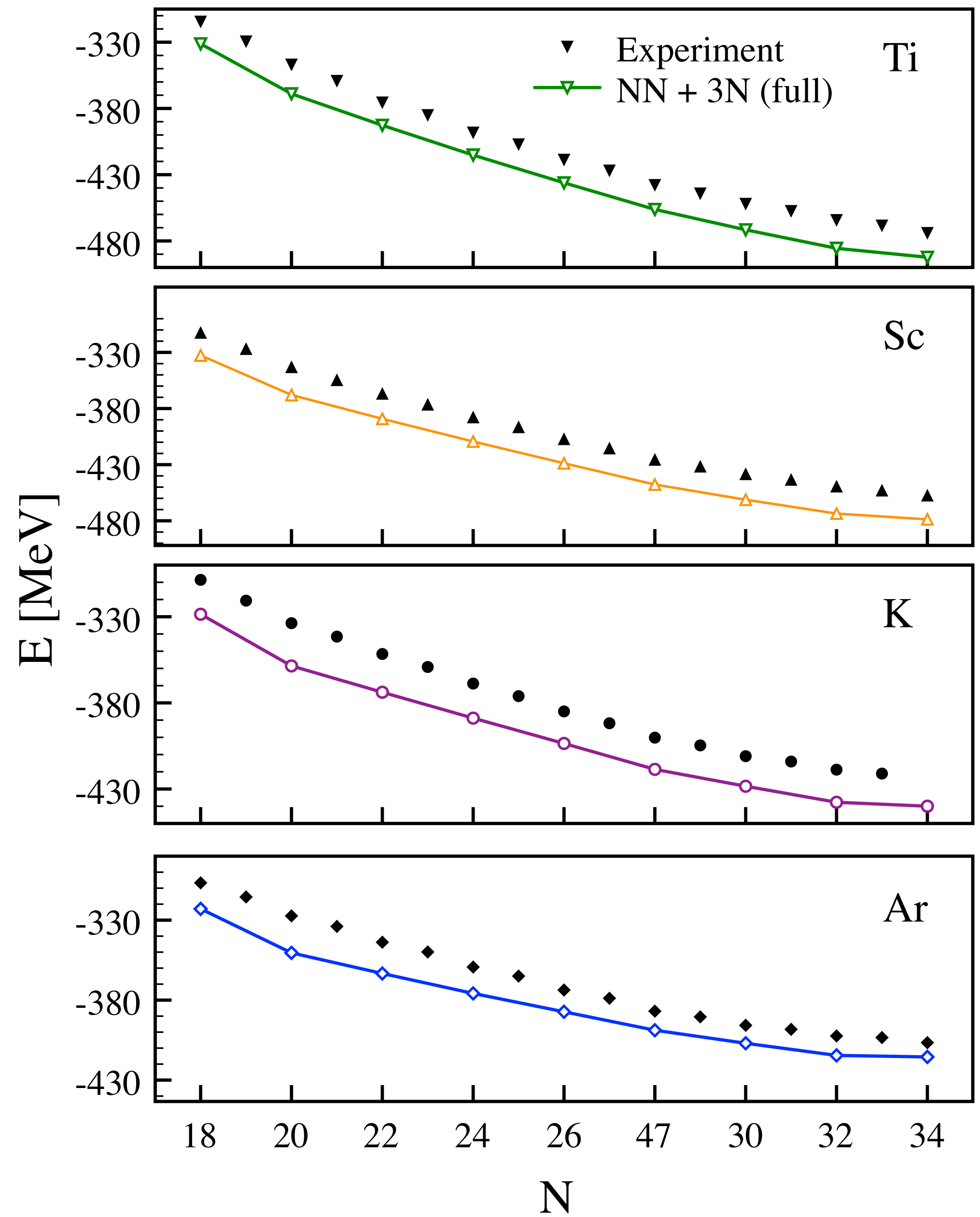


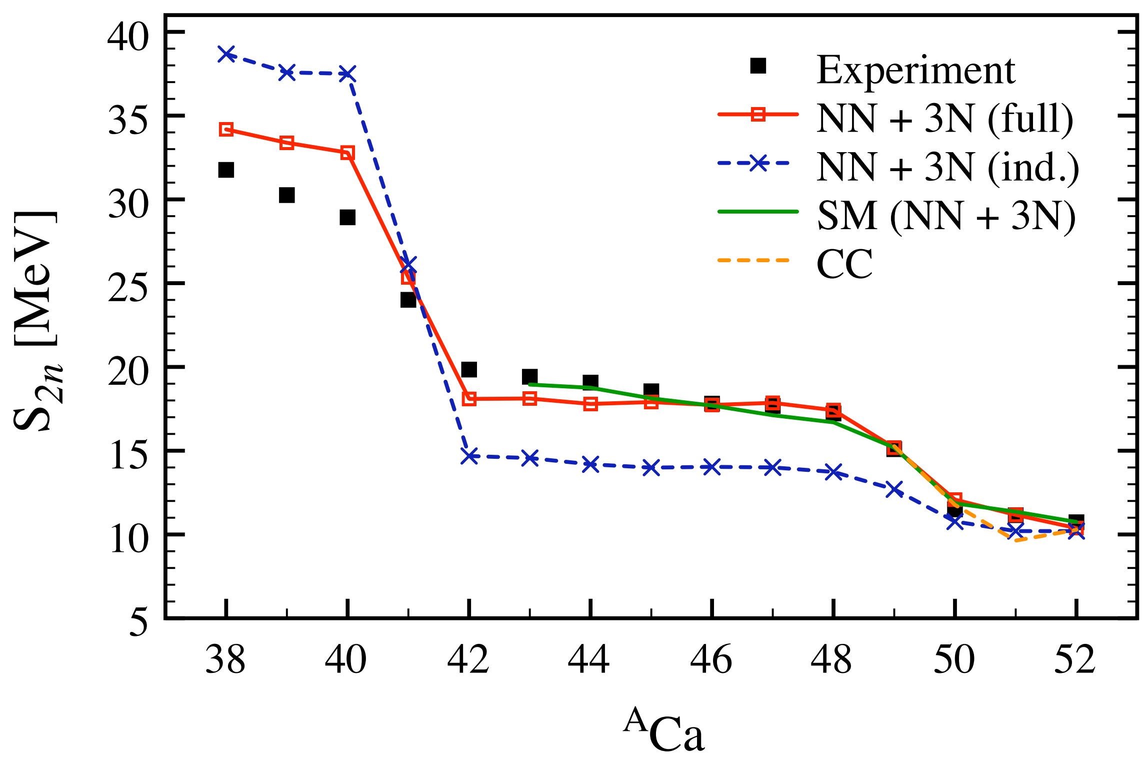


➟ Results confirmed within different many-body approaches

➟ NN + full 3N correct the trend of binding energies

➟ Systematic overbinding through all chains around Z=20

Two-neutron separation energies around Ca



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➠ Microscopic calculations extended to the whole Ca chain

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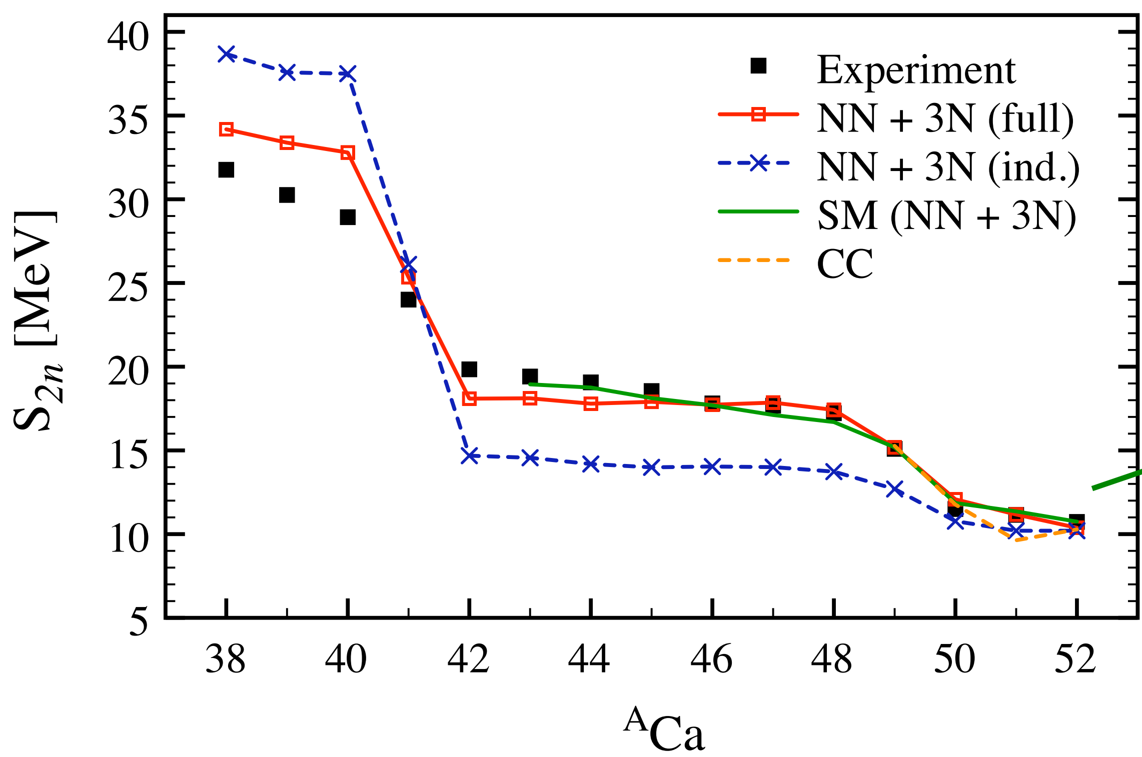

Challenging new data

[Gallant *et al*. 2012]

[Wienholtz *et al*. 2013]

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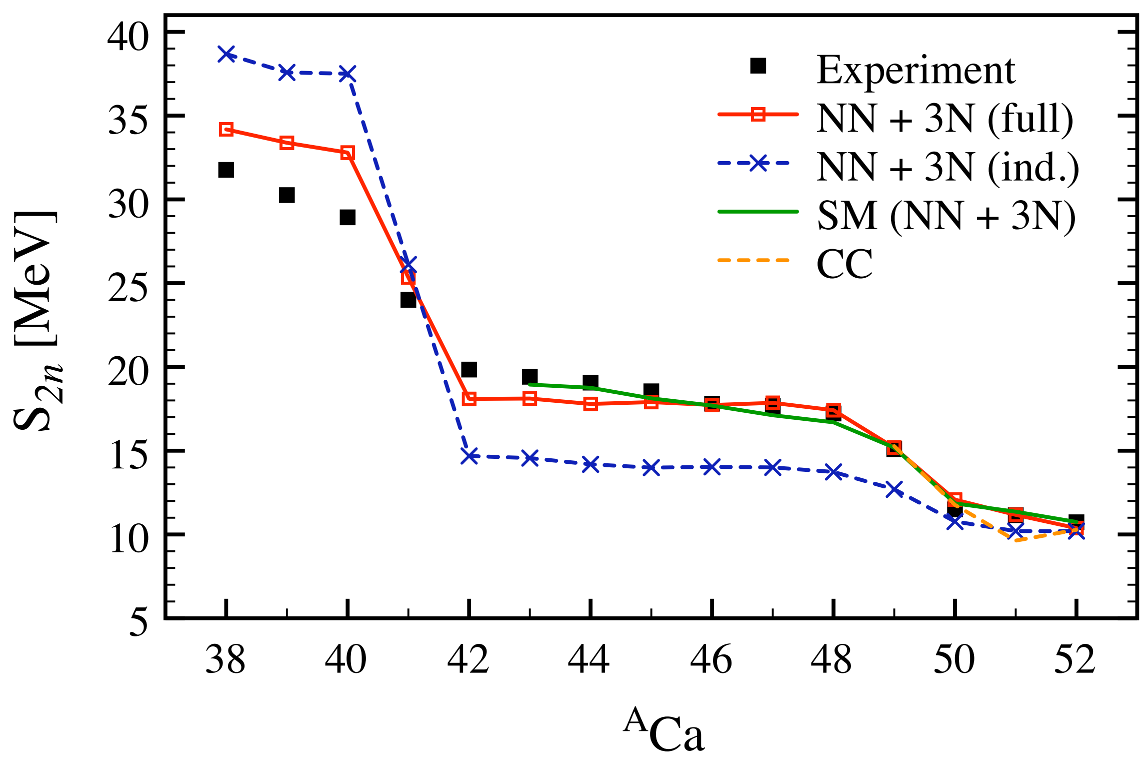

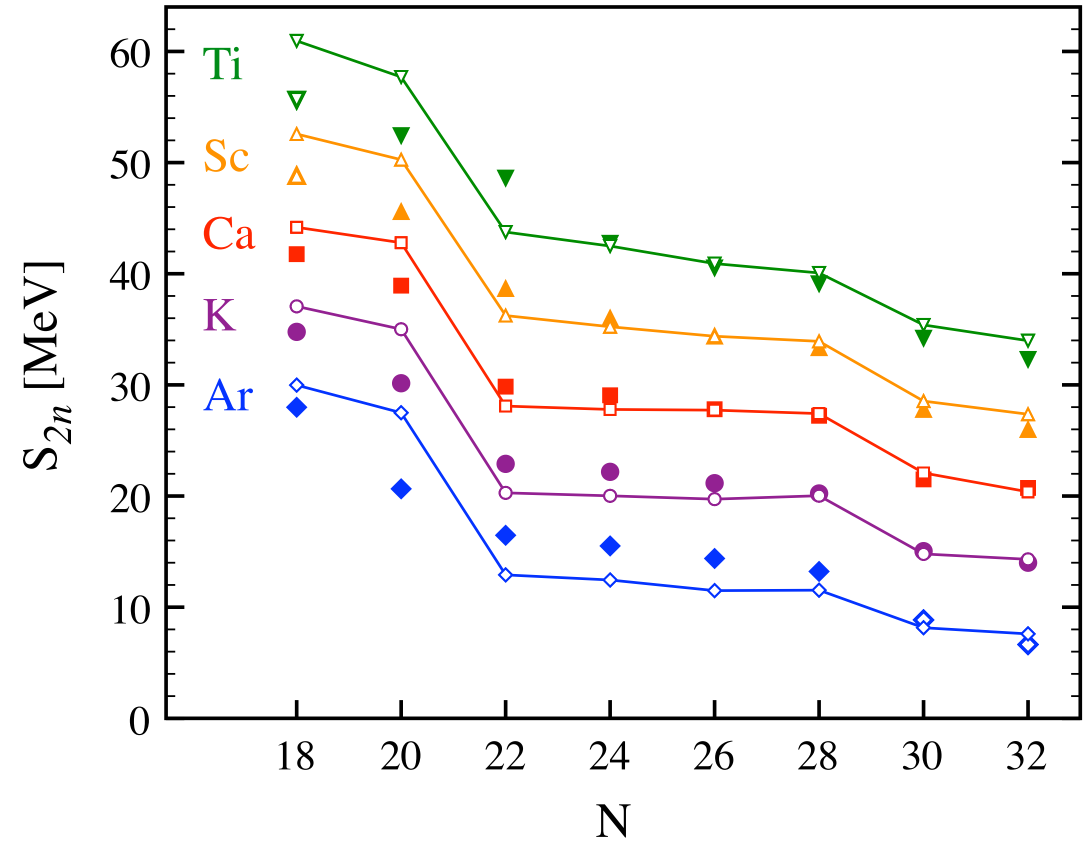

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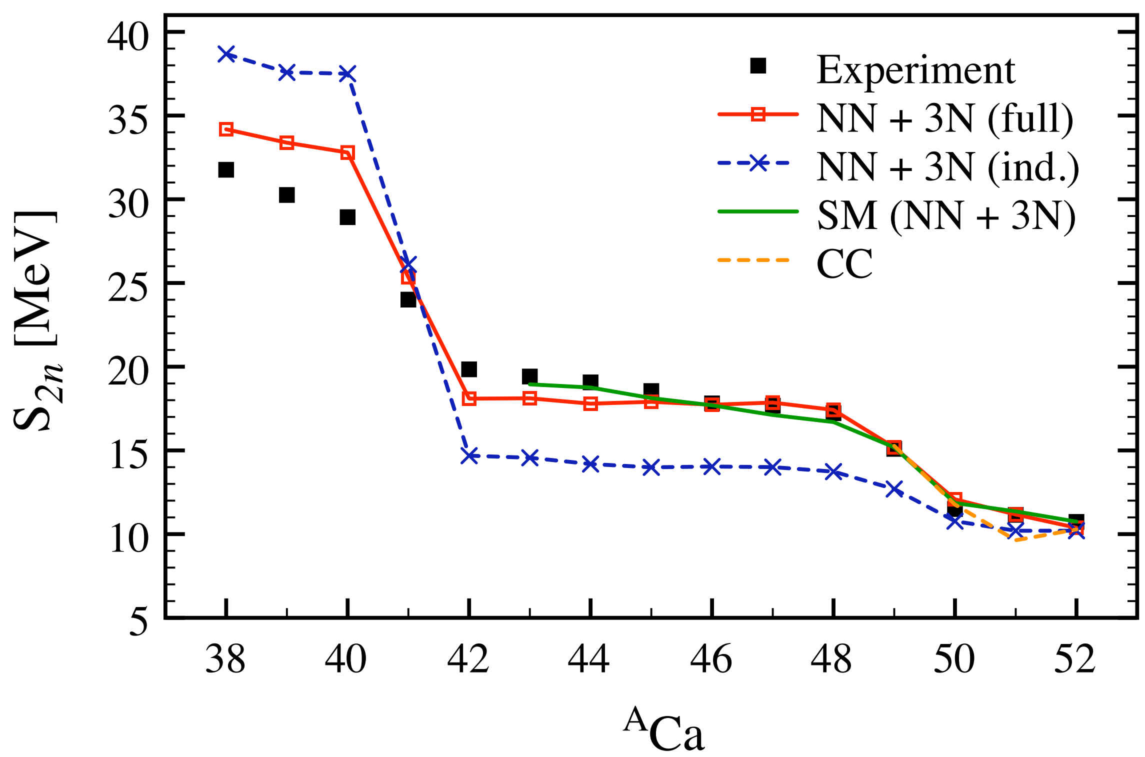

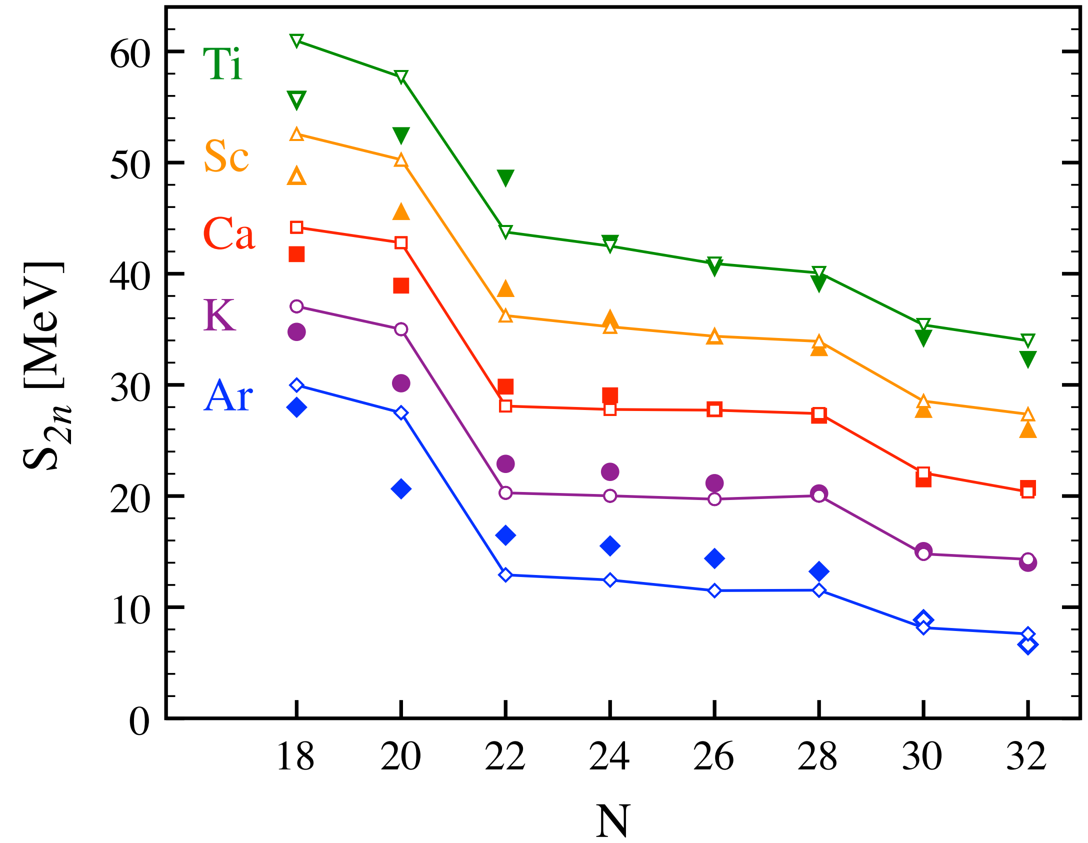

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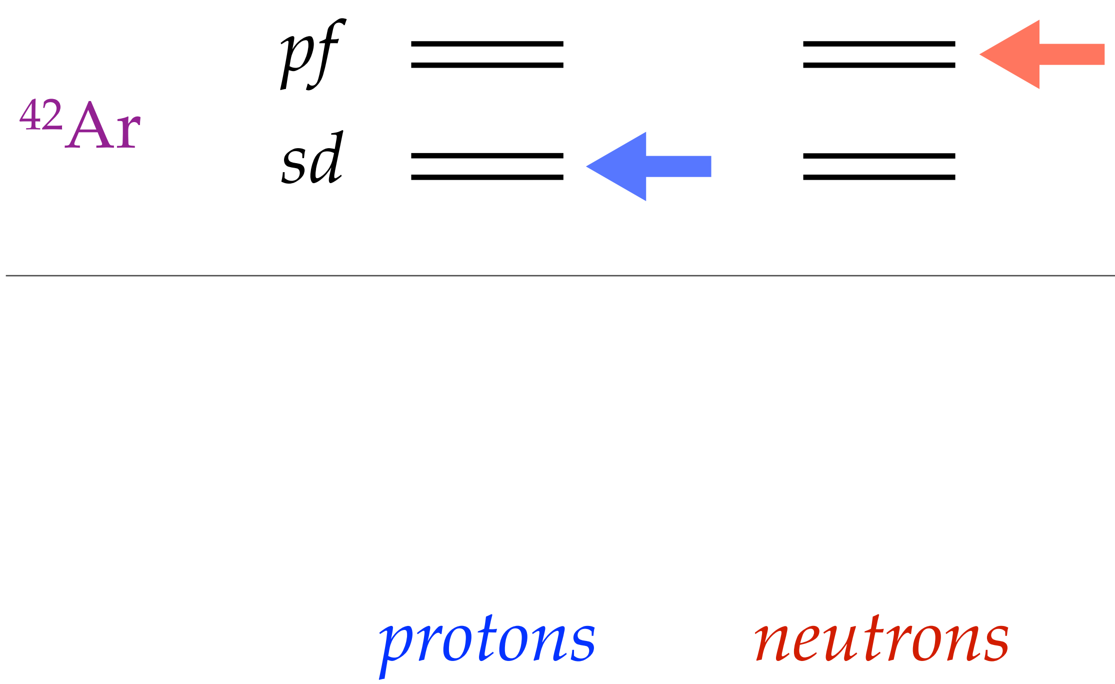

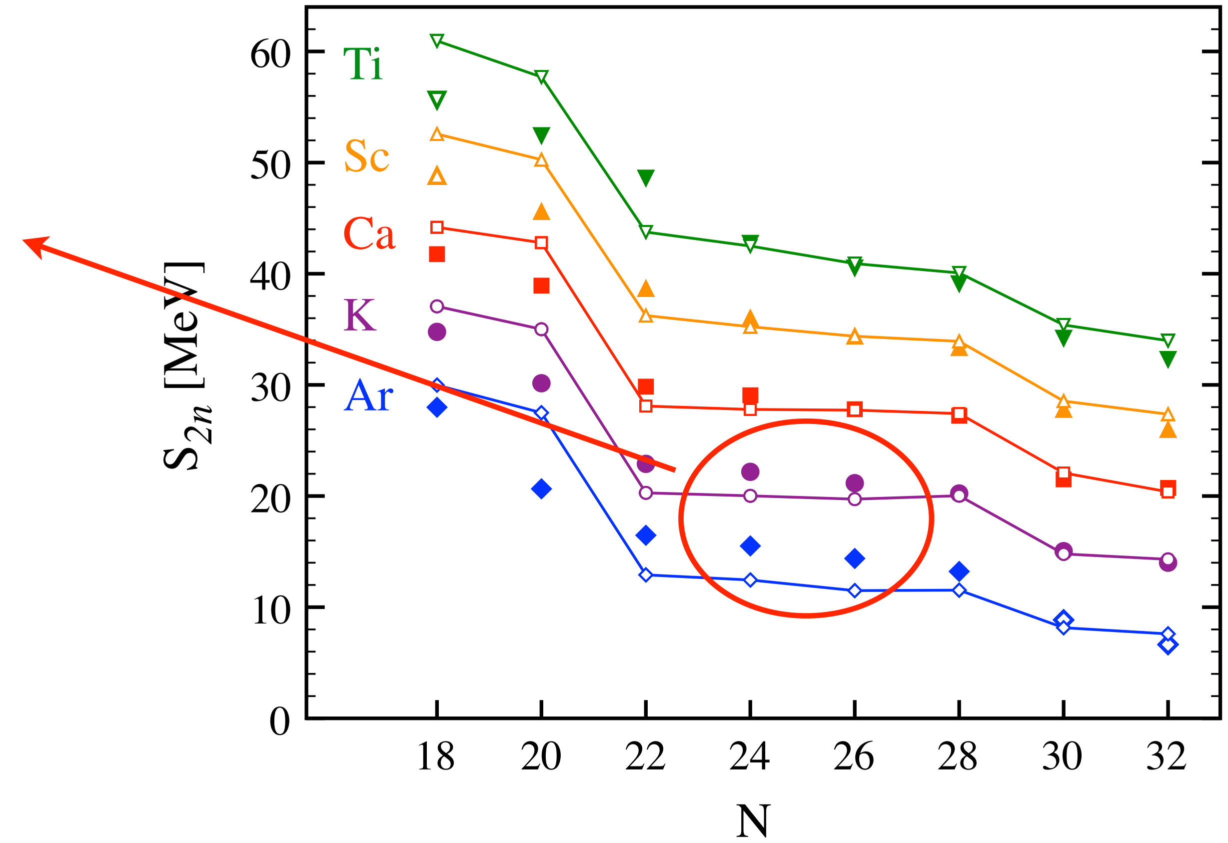

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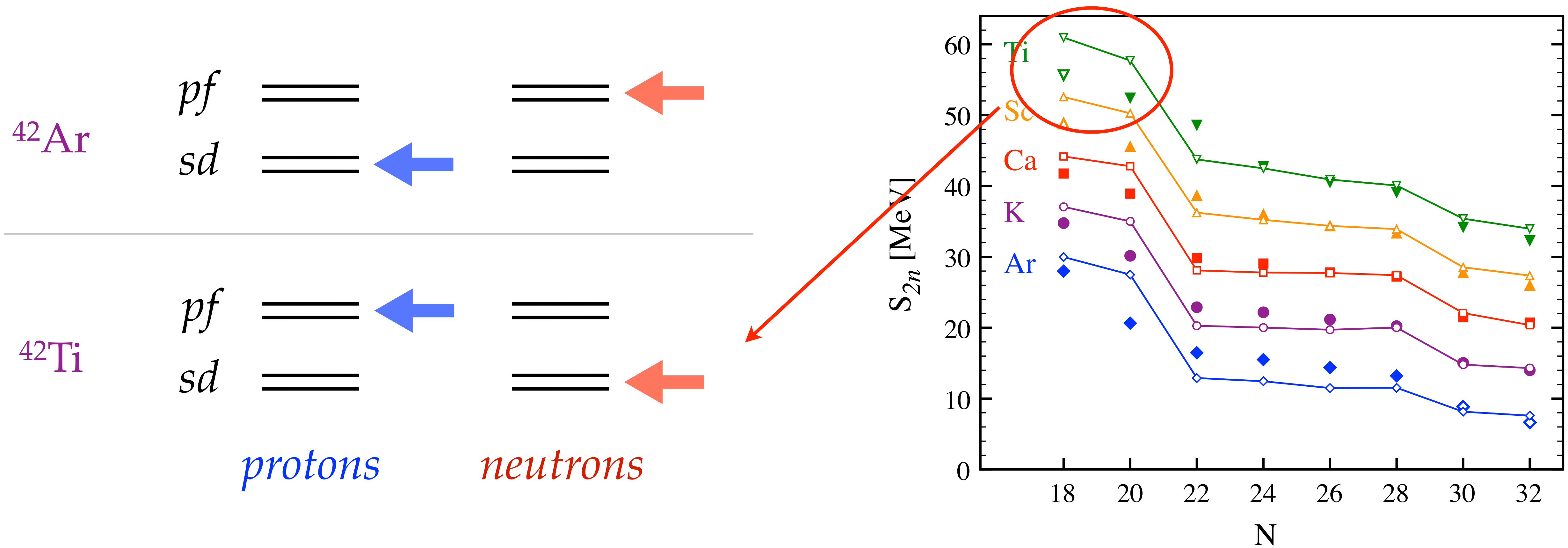

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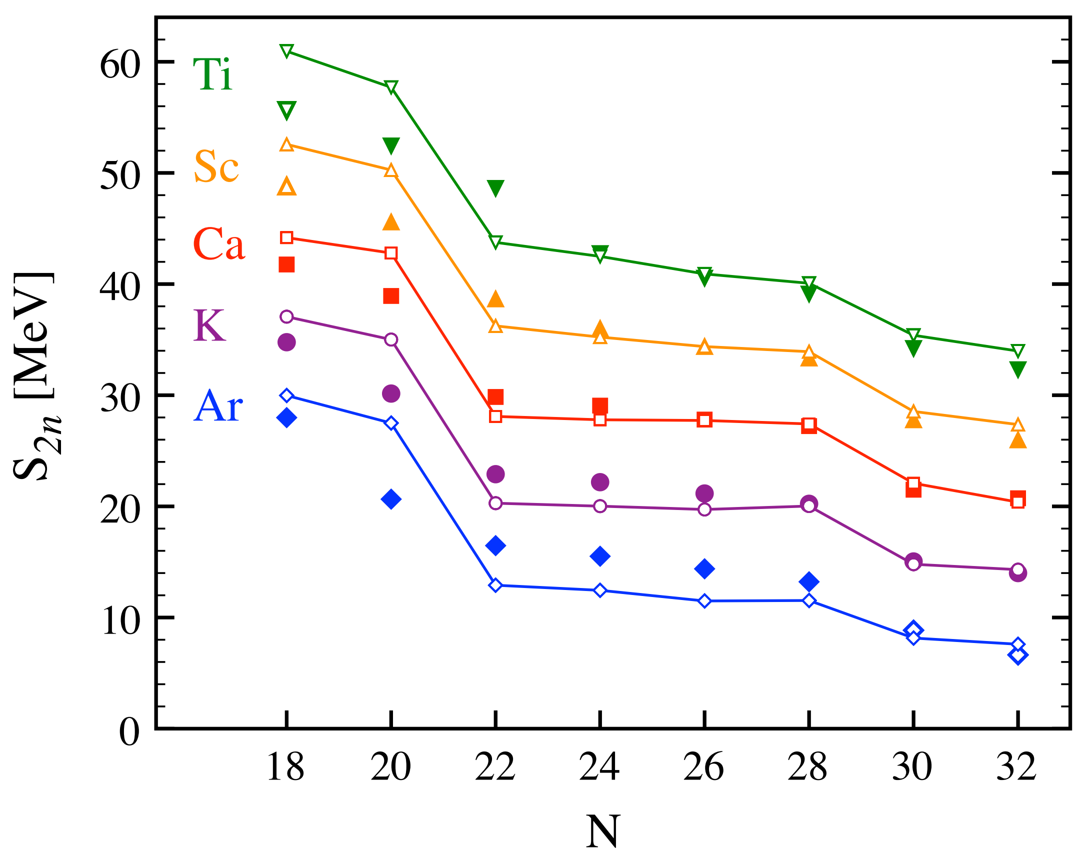
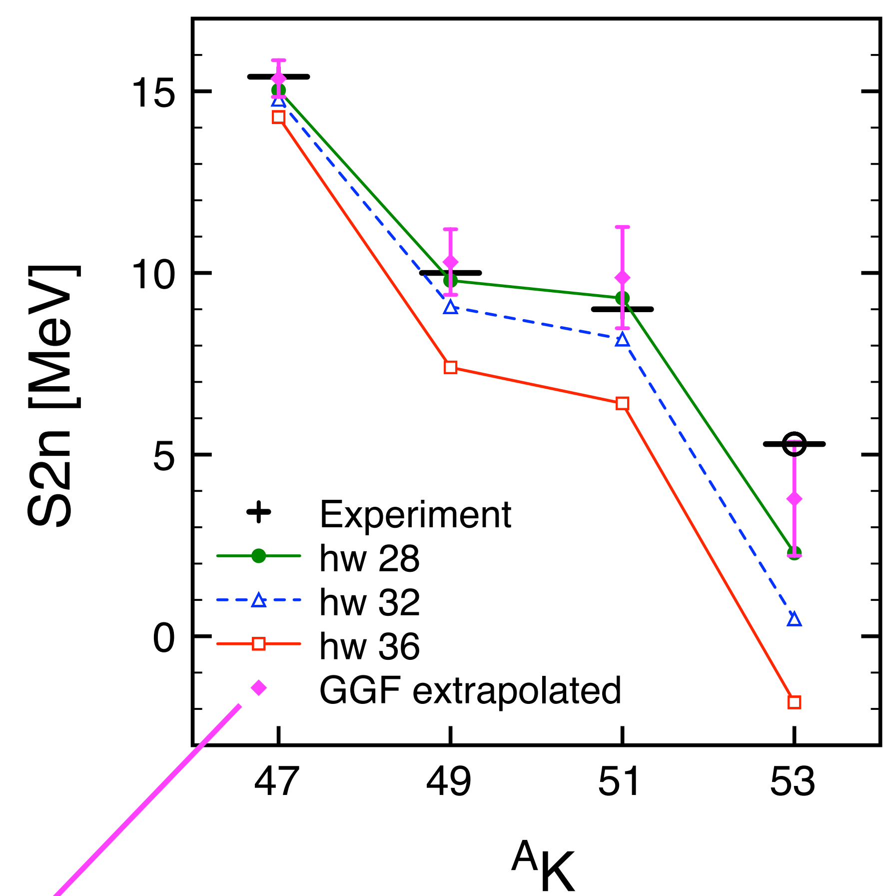
➟ Overestimation of N=20 gap traced back to spectrum too spread out

Extrapolation of the neutron-rich end

✪ Convergence worsens after N=32



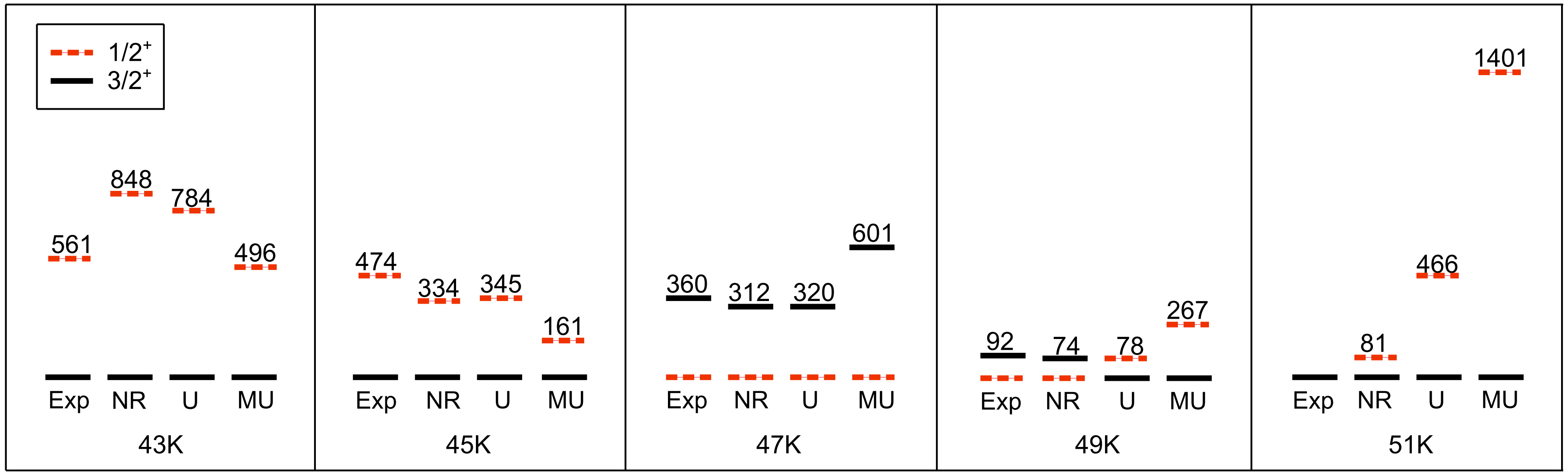


Extrapolation to infinite model space [Coon *et al.*, Furnstahl *et al.*]

Potassium ground states (re)inversion

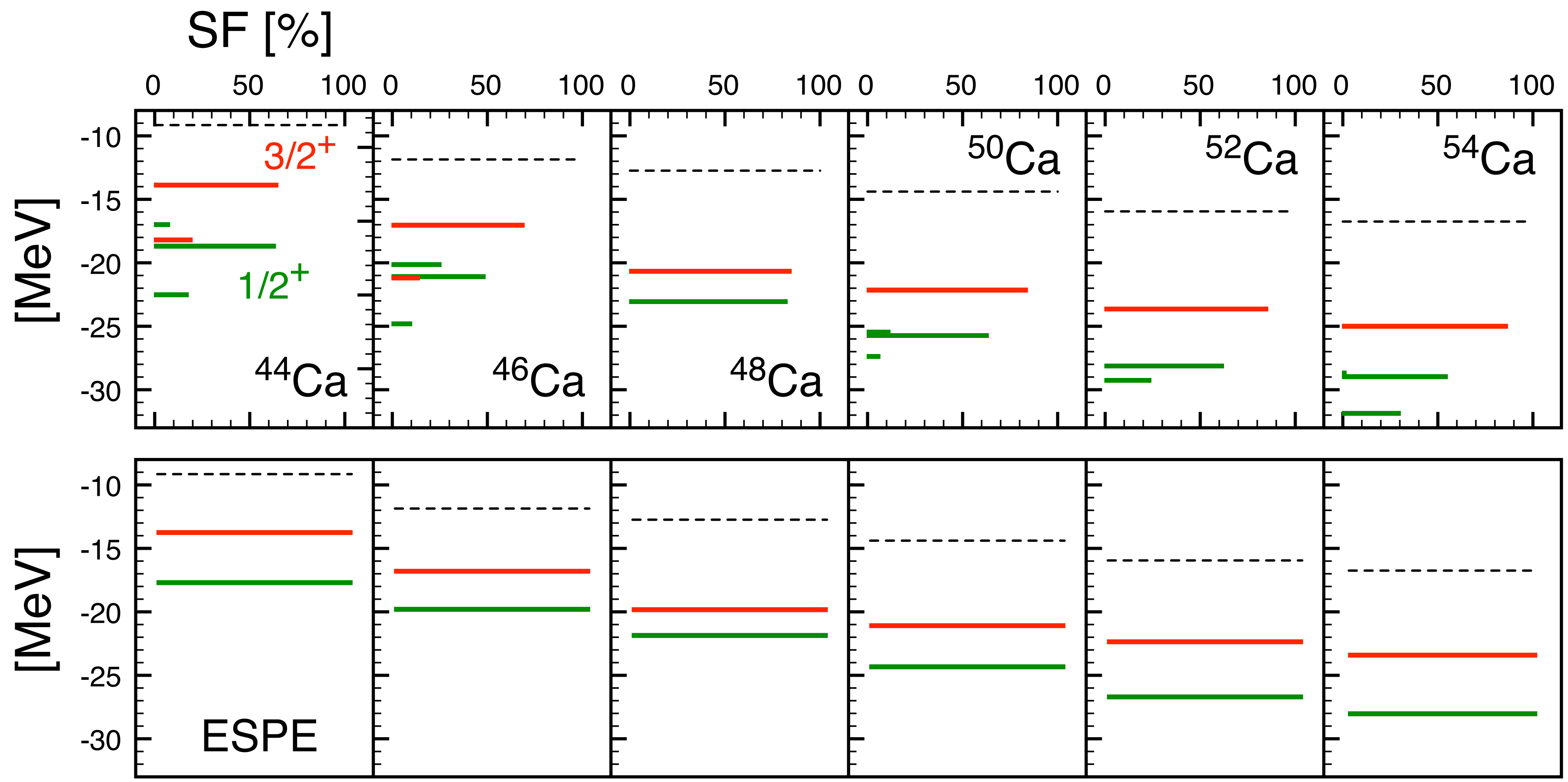
Laser spectroscopy
(@ ISOLDE)

[Papuga *et al.* 2013]



Theory (GGF)

[VS *et al.* unpublished]



Knockout & transfer experiments

✪ Neutron removal from proton- and neutron-rich Ar isotopes @ NSCL

Isotopes	lj^{π}	Sn(MeV)	ΔS (MeV)	(theo.) SF(LB-SM)	(expt.) SF(JLM + HF)	Rs(JLM + HF)	(expt.) SF(CH89)	Rs(CH89)
^{34}Ar	$s1/2^{+}$	17.07	12.41	1.31	0.85 ± 0.09	0.65 ± 0.07	1.10 ± 0.11	0.84 ± 0.08
^{36}Ar	$d3/2^{+}$	15.25	6.75	2.10	1.60 ± 0.16	0.76 ± 0.08	2.29 ± 0.23	1.09 ± 0.11
^{46}Ar	$f7/2^{-}$	8.07	−10.03	5.16	3.93 ± 0.39	0.76 ± 0.08	5.29 ± 0.53	1.02 ± 0.10

[Lee *et al.* 2010]

$\Delta S = Sn - Sp$

Gorkov GF NN

	Sn (MeV)	ΔS (MeV)	SF
^{34}Ar	33.0	18.6	1.46
^{36}Ar	27.7	7.5	1.46
^{46}Ar	16.0	-22.3	5.88

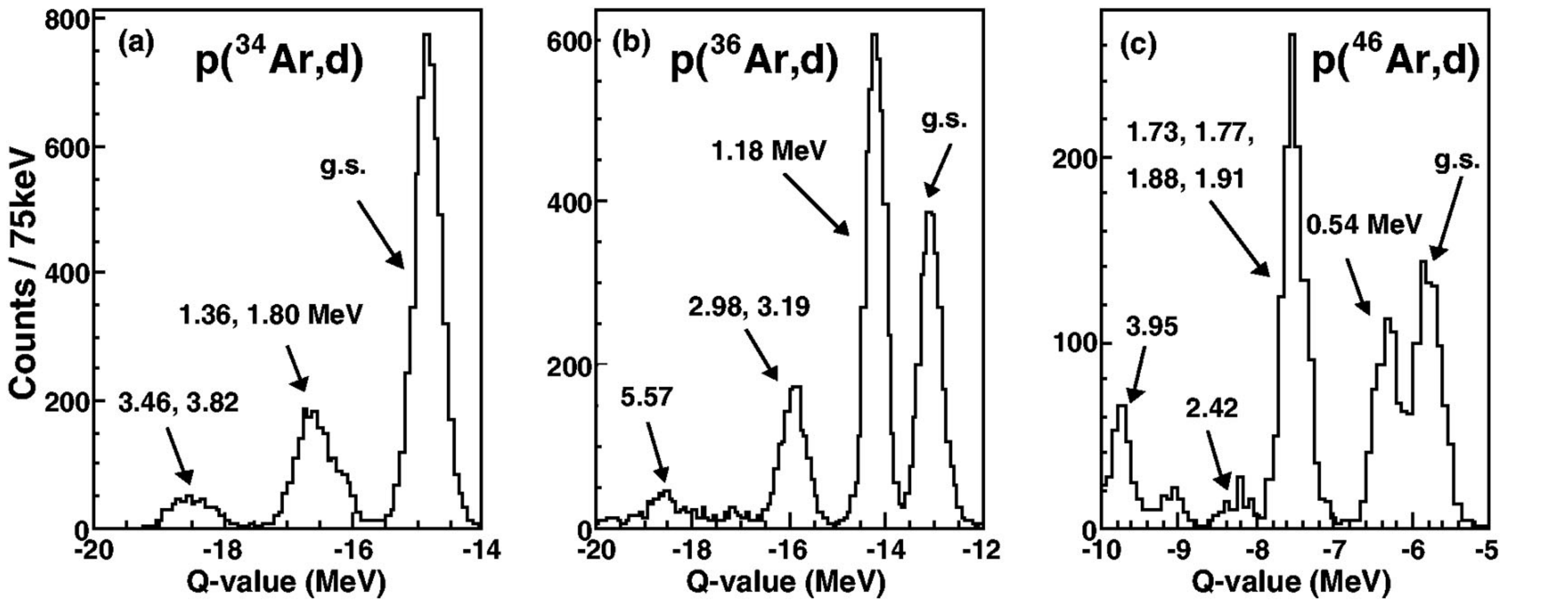
Gorkov GF NN + 3N

	Sn (MeV)	ΔS (MeV)	SF
^{34}Ar	22.4	15.5	1.56
^{36}Ar	15.3	7.2	1.54
^{46}Ar	6.5	-15.7	6.64

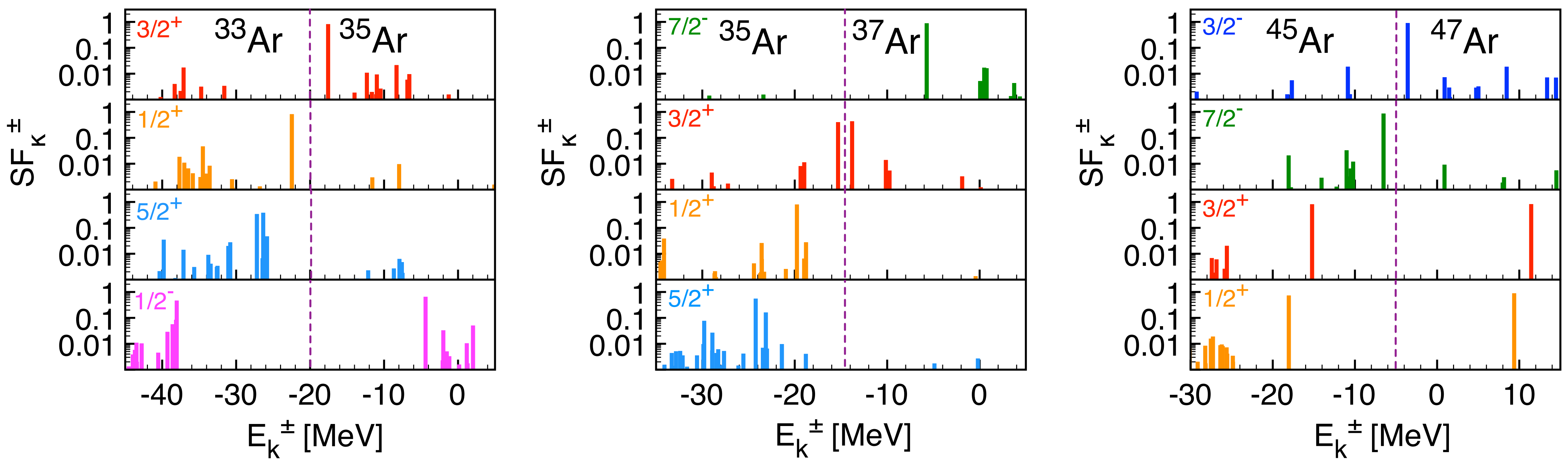
[VS *et al.* unpublished]

Knockout & transfer experiments

✪ Neutron removal from proton- and neutron-rich Ar isotopes @ NSCL



[Lee *et al.* 2010]



[VS *et al.* unpublished]

Summary & outlook

✪ Agreement between different many-body methods

➟ Model independent calculations challenge chiral interactions

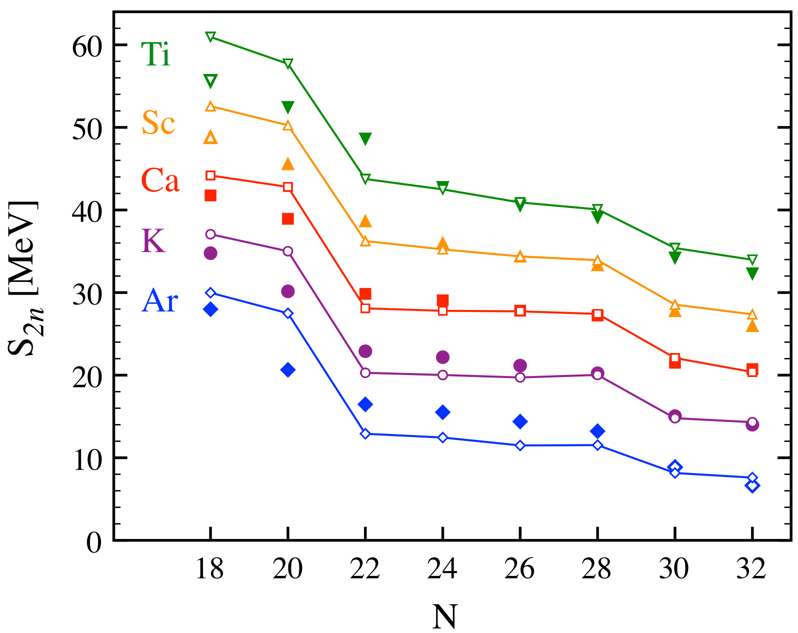
✪ Gorkov-Green's functions

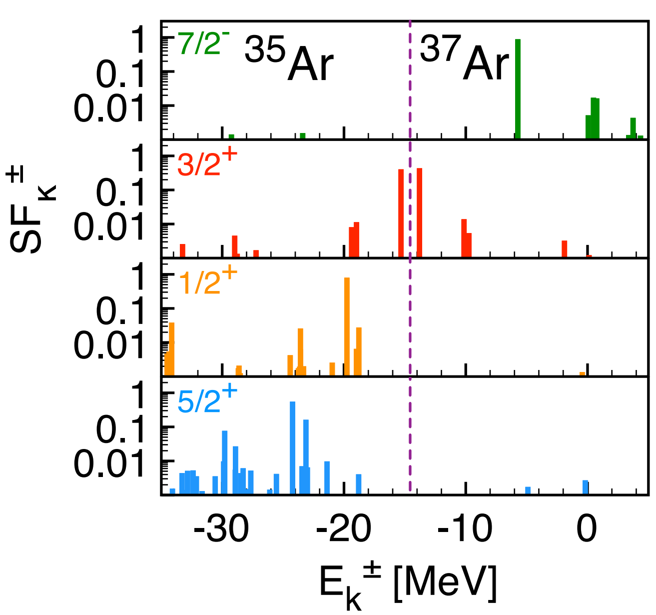
➟ Novel path to extend first-principle calculations to open-shells

➟ GGF(2) provides good reproduction of S2n around Ca

➟ Separation spectra at a qualitative level

➟ Work in progress: GGF(3)



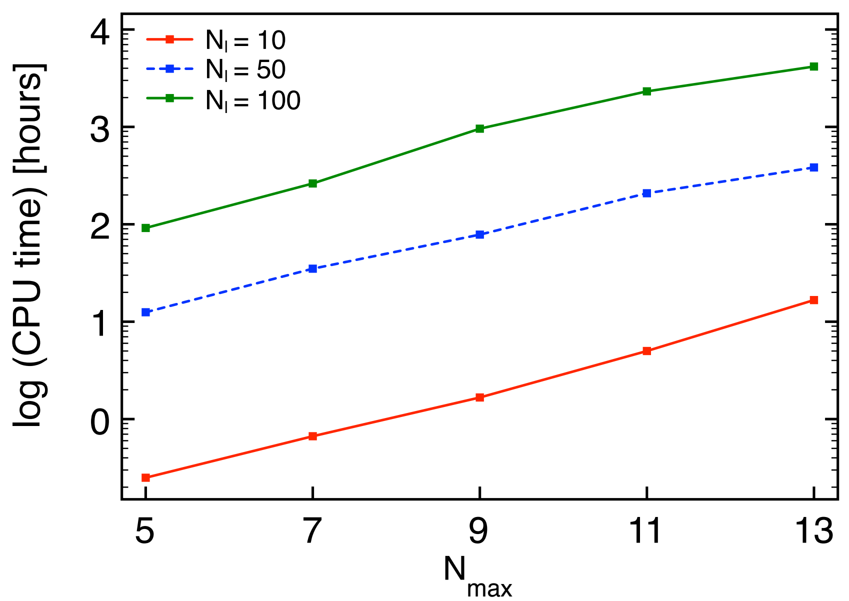


Appendix

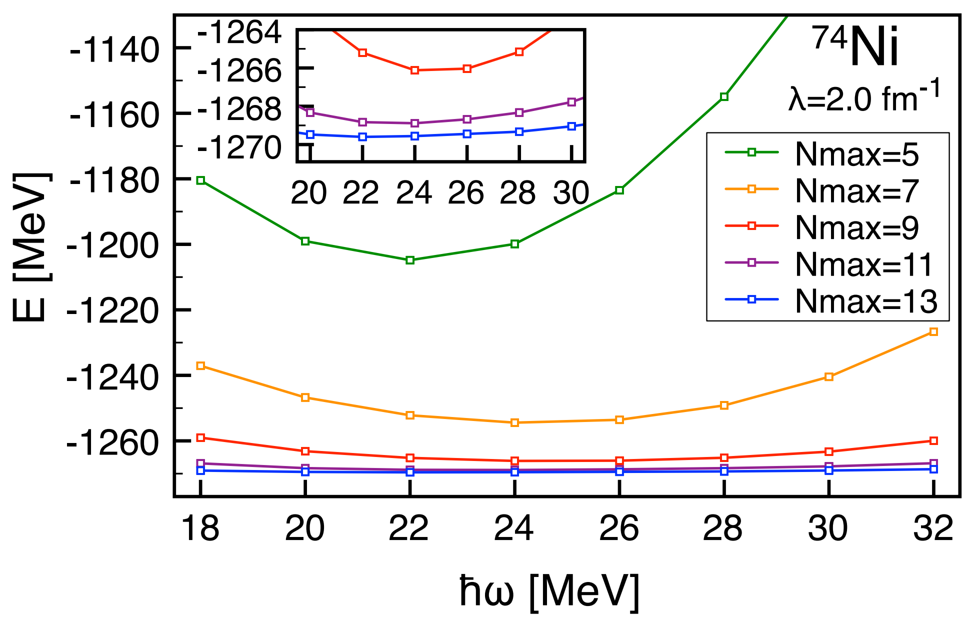
Scaling, convergence & theoretical errors

✪ Scaling and convergence thoroughly assessed

Scaling



Convergence



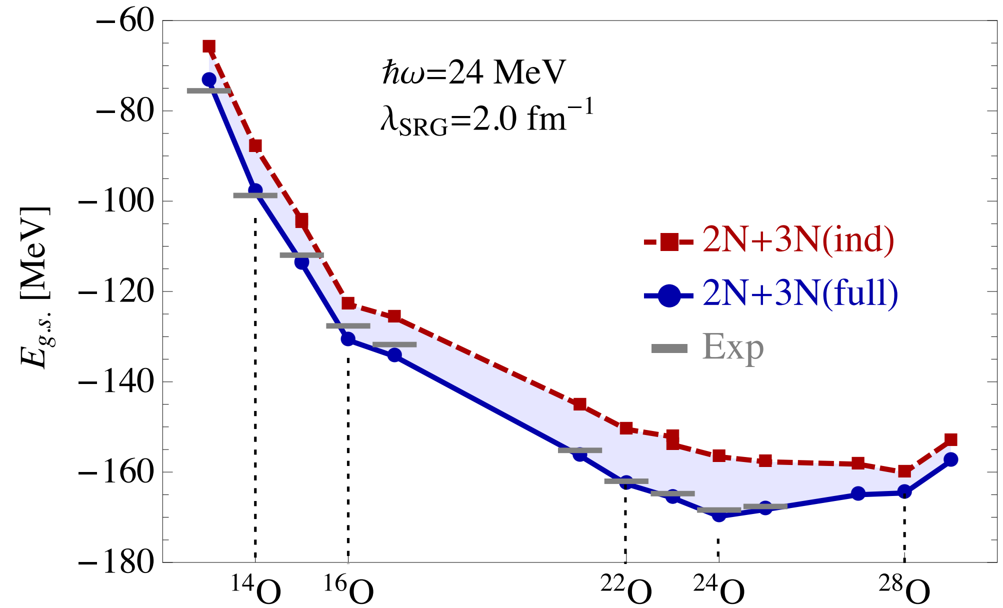
✪ Estimation of theoretical errors in *ab initio* methods

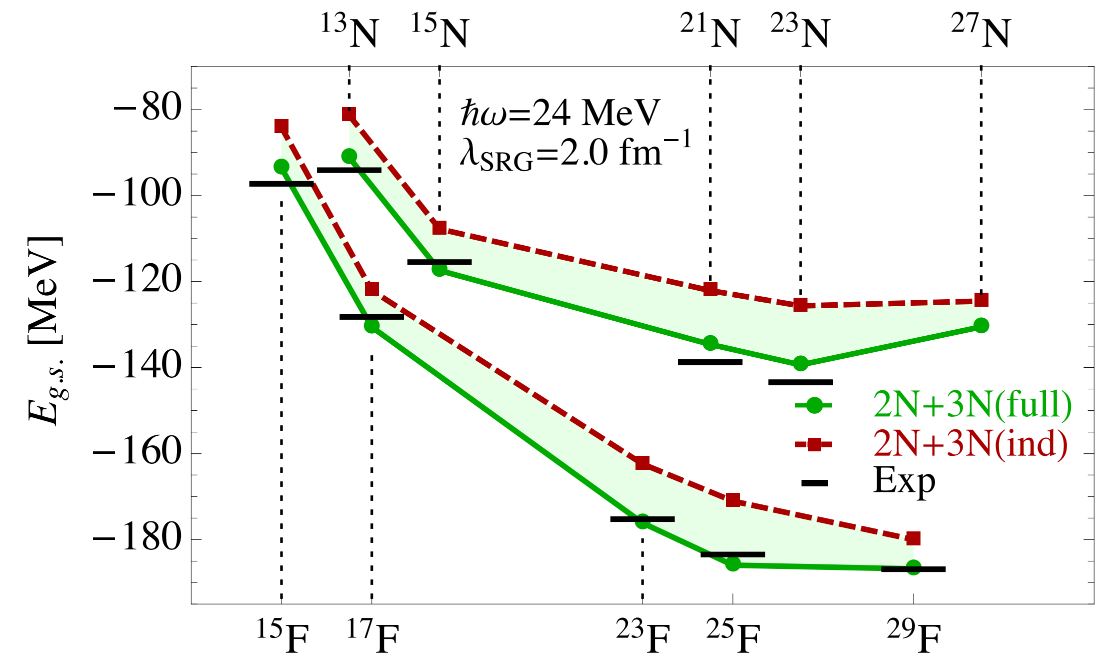
1) Hamiltonian	✘
2) Many-body expansion	✘/✔
3) Model space truncation	✔
4) Numerical algorithms	✔

⇐ GGF

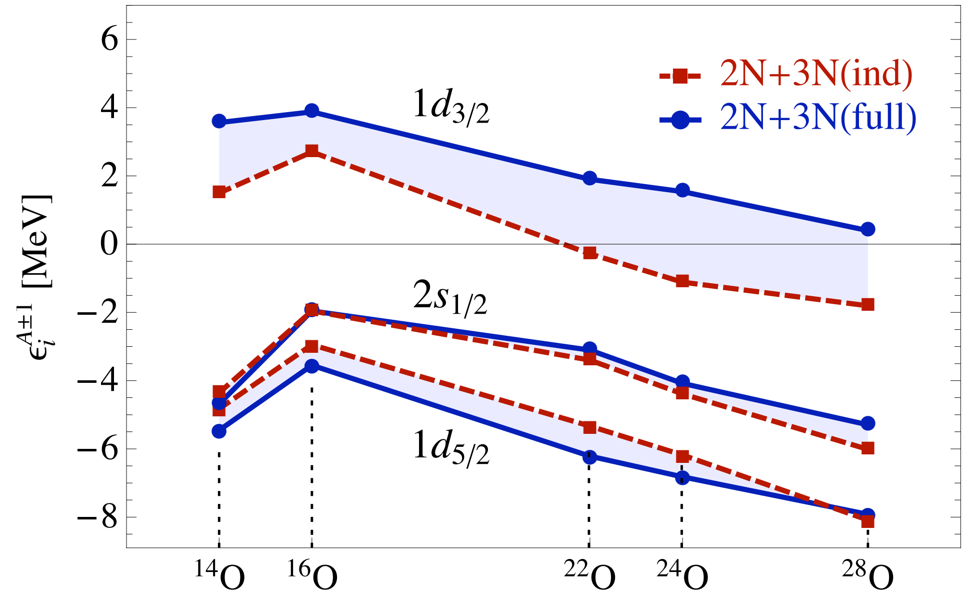
Not only oxygen...

✪ Consistent description of Z = 7, 8, 9 isotopic chains with GF method





[Cipollone, Barbieri & Navrátil 2013]



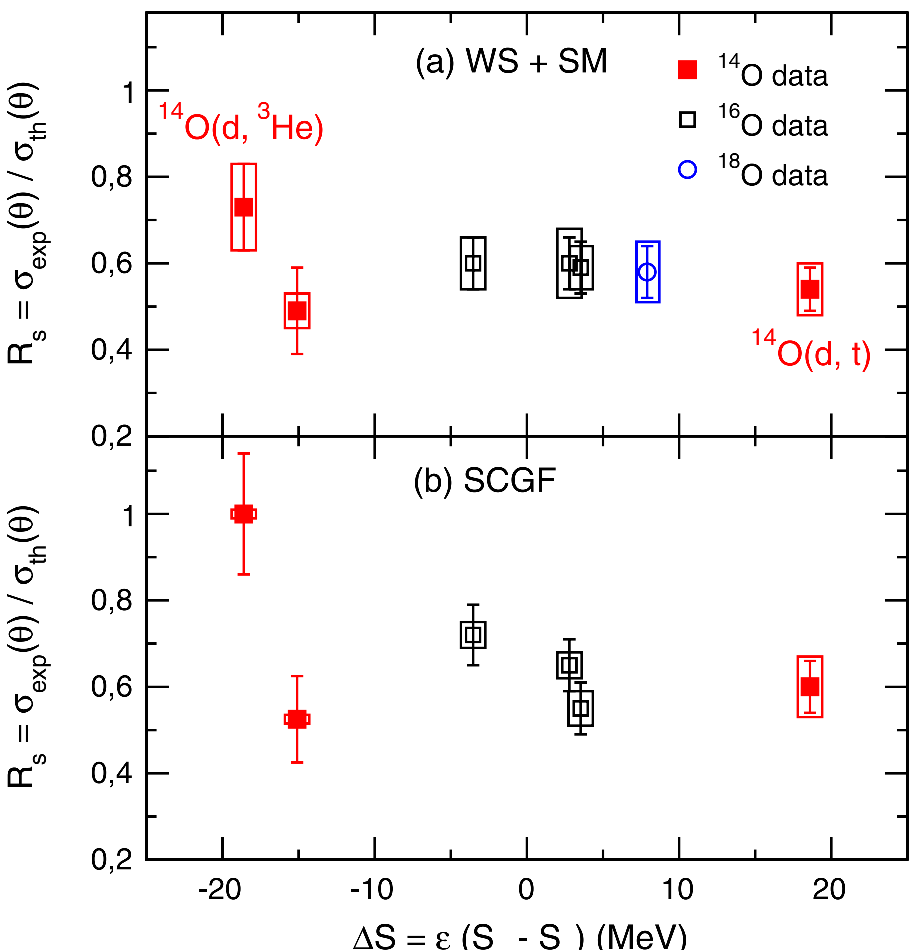
➠ 3NF crucial for reproducing driplines

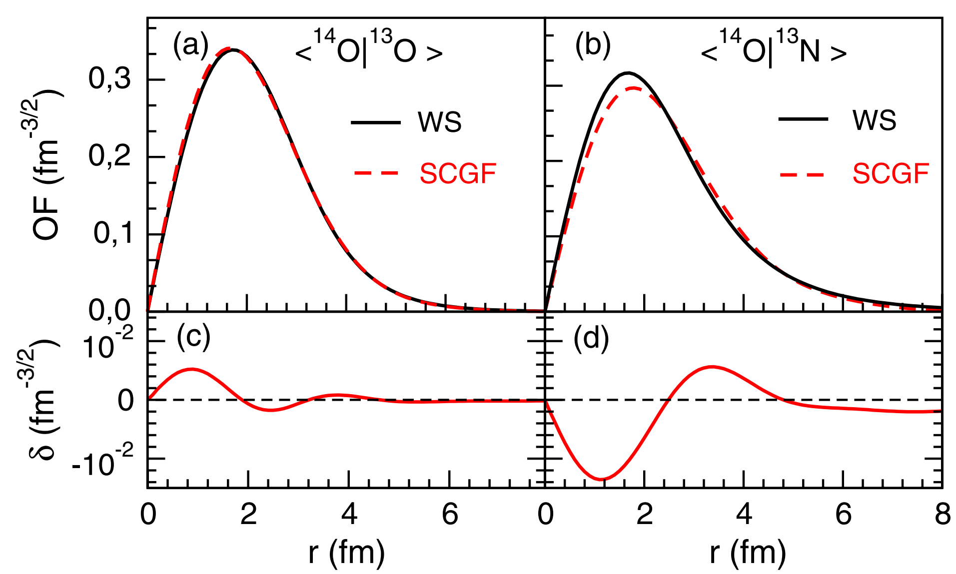
➠ $d_{3/2}$ raised by genuine 3NF

Single-nucleon transfer in the oxygen chain

✪ Analysis of $^{14}O(d,t)\,^{13}O$ and $^{14}O(d,{}^{3}He)\,^{13}N$ transfer reactions @ SPIRAL

Reaction	E^* (MeV)	J^π	R_{rms}^{HFB} (fm)	r_0 (fm)	C^2S_{exp} (WS)	C^2S_{th} $0p+2\hbar\omega$	R_s (WS)	C^2S_{exp} (SCGF)	C^2S_{th} (SCGF)	R_s (SCGF)
^{14}O (d,t) ^{13}O	0.00	$3/2^-$	2.69	1.40	1.69 (17)(20)	3.15	0.54(5)(6)	1.89(19)(22)	3.17	0.60(6)(7)
^{14}O $(d,{}^{3}He)$ ^{13}N	0.00	$1/2^-$	3.03	1.23	1.14(16)(15)	1.55	0.73(10)(10)	1.58(22)(2)	1.58	1.00(14)(1)
	3.50	$3/2^-$	2.77	1.12	0.94(19)(7)	1.90	0.49(10)(4)	1.00(20)(1)	1.90	0.53(10)(1)
^{16}O (d,t) ^{15}O	0.00	$1/2^-$	2.91	1.46	0.91(9)(8)	1.54	0.59(6)(5)	0.96(10)(7)	1.73	0.55(6)(4)
^{16}O $(d,{}^{3}He)$ ^{15}N [19,20]	0.00	$1/2^-$	2.95	1.46	0.93(9)(9)	1.54	0.60(6)(6)	1.25(12)(5)	1.74	0.72(7)(3)
	6.32	$3/2^-$	2.80	1.31	1.83(18)(24)	3.07	0.60(6)(8)	2.24(22)(10)	3.45	0.65(6)(3)
^{18}O $(d,{}^{3}He)$ ^{17}N [21]	0.00	$1/2^-$	2.91	1.46	0.92(9)(12)	1.58	0.58(6)(10)			





➟ Overlaps functions and cross sections from GF

➟ R_s independent of asymmetry

[Flavigny *et al.* 2013]