

Masses, spectra and radii from SCGF calculations

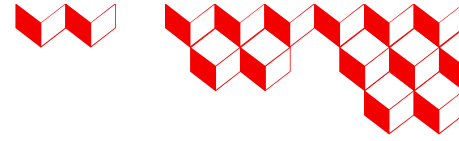
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ESNT workshop “Ab initio many-body calculations: where has the nuclear pairing gone?”

20 May 2025

Outline



0. Reminder of self-consistent Green's functions (SCGF) formalism

1. Breaking particle number: Gorkov SCGF

- Gorkov algebraic diagrammatic construction (ADC)
- Binding energies
- Excitation spectra
- Charge radii

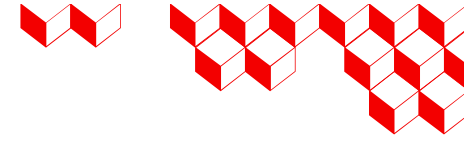
2. Breaking rotational invariance: deformed SCGF

- Recent developments & preliminary results

3. Perspectives

- Gorkov ADC(3) & dimensionality-reduction techniques

Self-consistent Green's function approach



A-body wave function

$$|\Psi_k^A\rangle$$



A-body Schrödinger equation

$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$$



Observables: exp. values

$$O = \langle \Psi_0^A | O | \Psi_0^A \rangle$$

Green's functions

$$\begin{aligned} i g_{\alpha\beta}(t_\alpha, t_\beta) &\equiv \langle \Psi_0^A | \mathcal{T}[a_\alpha(t_\alpha) a_\beta^\dagger(t_\beta)] | \Psi_0^A \rangle \\ i g_{\alpha\gamma\beta\delta}^{4\text{-pt}}(t_\alpha, t_\gamma, t_\beta, t_\delta) &\equiv \langle \Psi_0^A | \mathcal{T}[a_\gamma(t_\gamma) a_\alpha(t_\alpha) a_\beta^\dagger(t_\beta) a_\delta^\dagger(t_\delta)] | \Psi_0^A \rangle \\ &\dots \end{aligned}$$

Dyson equation

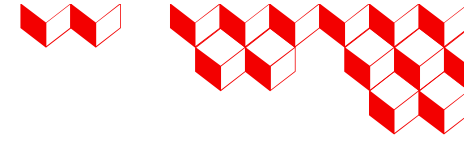
$$g_{\alpha\beta}(\omega) = g_{0\alpha\beta}(\omega) + \sum_{\gamma\delta} g_{0\alpha\gamma}(\omega) \Sigma_{\gamma\delta}^*(\omega) g_{\delta\beta}(\omega)$$

Self-energy expansion \rightarrow Many-body approximations $\xrightarrow{\text{e.g.}}$ ADC(n)

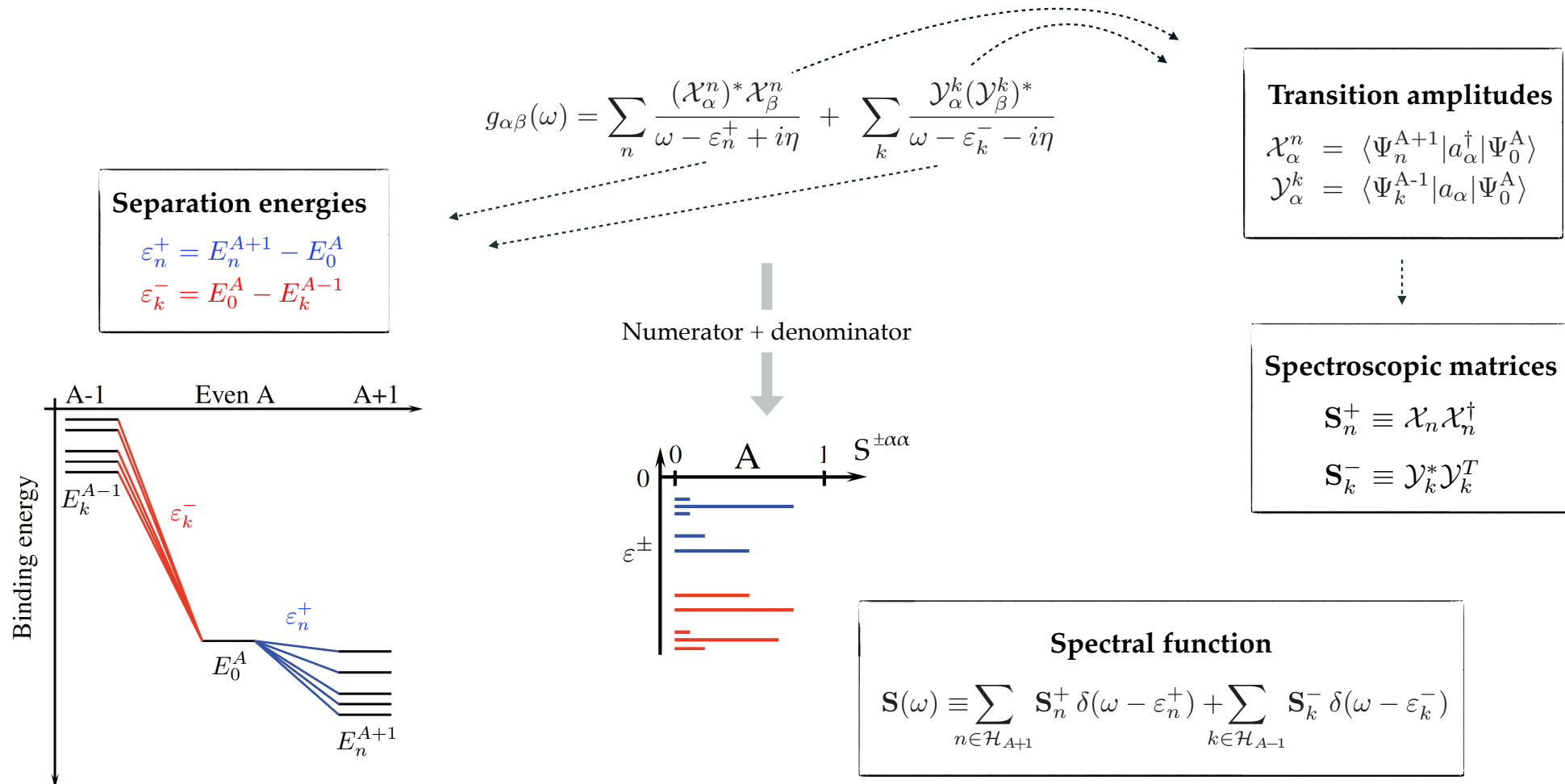
Observables: convolutions with GFs

$$\langle \Psi_0^A | O^{1B} | \Psi_0^A \rangle = \sum_{\alpha\beta} \int \frac{d\omega}{2\pi i} g_{\beta\alpha}(\omega) o_{\alpha\beta}$$

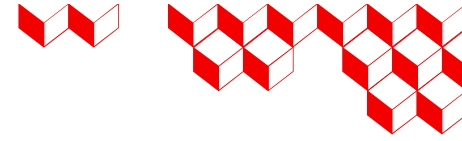
Spectral representation



- One-body propagator displays **spectral representation (Kallén-Lehmann)**



Self-energy expansion



- Exact self-energy can be expanded and decomposed as

$$\Sigma_{\alpha\beta}^*(\omega) = \Sigma_{\alpha\beta}^{(n=1)}(\omega) + \Sigma_{\alpha\beta}^{(n>1)}(\omega) \equiv \Sigma_{\alpha\beta}^{(\infty)} + \tilde{\Sigma}_{\alpha\beta}(\omega)$$

- Dynamic** (energy-dependent) self-energy also displays a spectral representation

$$\tilde{\Sigma}_{\alpha\beta}(\omega) = \sum_j \frac{\mathcal{M}_{\alpha j}^\dagger \mathcal{M}_{j\beta}}{\omega - \mathcal{E}_j^+ + i\eta} + \sum_k \frac{\mathcal{N}_{\alpha k} \mathcal{N}_{k\beta}^\dagger}{\omega - \mathcal{E}_k^- - i\eta}$$

A+1 configurations
A-1 configurations

Dyson eq. in matrix form

$$\varepsilon_i \begin{pmatrix} \mathcal{Z}_\alpha^i \\ \mathcal{W}_j^i \\ \mathcal{W}_k^i \end{pmatrix} = \begin{pmatrix} h_{\alpha\delta}^{(0)} + \Sigma_{\alpha\delta}^{(\infty)} & \mathcal{M}_{\alpha j}^\dagger & \mathcal{N}_{\alpha k} \\ \mathcal{M}_{j\delta} & \mathcal{E}_j^+ & 0 \\ \mathcal{N}_{k\delta}^\dagger & 0 & \mathcal{E}_k^- \end{pmatrix} \begin{pmatrix} \mathcal{Z}_\delta^i \\ \mathcal{W}_j^i \\ \mathcal{W}_k^i \end{pmatrix}$$

- Self-energy approximated via the **Algebraic Diagrammatic Construction (ADC)**

1. Rewrite exact self-energy as

$$\tilde{\Sigma}_{\alpha\beta}^{(\text{ADC})}(\omega) = \sum_{jj'} M_{\alpha j}^\dagger \left[\frac{1}{\omega \mathbb{1} - \underbrace{(E^> + C)}_{\text{Non-diagonal energy matrices}} + i\eta \mathbb{1}} \right]_{jj'} M_{j'\beta} + \sum_{kk'} N_{\alpha k} \left[\frac{1}{\omega \mathbb{1} - \underbrace{(E^< + D)}_{\text{Non-diagonal energy matrices}} - i\eta \mathbb{1}} \right]_{kk'} N_{k'\beta}^\dagger$$

[Schirmer 1982]

- Expand M , N , C & D in perturbation → Combine them to construct ADC at order n , i.e. **ADC(n)**
- Determine M , N , C & D by requiring that ADC(n) contains standard **perturbative expansion up to order n**

Gorkov SCGF



⊙ Breaking **particle-number symmetry** → Efficient way to incorporate **pairing** correlations → Description of singly **open-shell nuclei**

Symmetry-breaking wave function

$$|\Psi_0\rangle = \sum_A^{\text{even}} |\Psi_0^A\rangle$$

[Gorkov 1958]

[Somà, Duguet, Barbieri 2011]

Generalised one-body GFs

$$\begin{aligned} i g_{\alpha\beta}^{11}(t-t') &\equiv \langle \Psi_0 | T[a_\alpha(t) a_\beta^\dagger(t')] | \Psi_0 \rangle \\ i g_{\alpha\beta}^{12}(t-t') &\equiv \langle \Psi_0 | T[a_\alpha(t) \bar{a}_\beta(t')] | \Psi_0 \rangle \\ i g_{\alpha\beta}^{21}(t-t') &\equiv \langle \Psi_0 | T[\bar{a}_\alpha^\dagger(t) a_\beta^\dagger(t')] | \Psi_0 \rangle \\ i g_{\alpha\beta}^{22}(t-t') &\equiv \langle \Psi_0 | T[\bar{a}_\alpha^\dagger(t) \bar{a}_\beta(t')] | \Psi_0 \rangle \end{aligned}$$

Nambu notation

$$\begin{aligned} i \mathbf{g}_{\alpha\beta}(t-t') &\equiv \langle \Psi_0 | T \{ \mathbf{A}_\alpha(t) \mathbf{A}_\beta^\dagger(t') \} | \Psi_0 \rangle \\ &= i \begin{pmatrix} g_{\alpha\beta}^{11}(t-t') & g_{\alpha\beta}^{12}(t-t') \\ g_{\alpha\beta}^{21}(t-t') & g_{\alpha\beta}^{22}(t-t') \end{pmatrix} \end{aligned}$$

Spectral representation

$$\mathbf{g}_{\alpha\beta}(\omega) = \sum_k \left\{ \frac{\mathbf{X}_\alpha^k \mathbf{X}_\beta^{k\dagger}}{\omega - \omega_k + i\eta} + \frac{\mathbf{Y}_\alpha^k \mathbf{Y}_\beta^{k\dagger}}{\omega + \omega_k - i\eta} \right\}$$

Gorkov equation

$$\mathbf{g}_{\alpha\beta}(\omega) = \mathbf{g}_{0\alpha\beta}(\omega) + \sum_{\gamma\delta} \mathbf{g}_{0\alpha\gamma}(\omega) \Sigma_{\gamma\delta}^*(\omega) \mathbf{g}_{\gamma\beta}(\omega)$$

$$\Sigma_{\alpha\beta}^*(\omega) \equiv \begin{pmatrix} \Sigma_{\alpha\beta}^{*11}(\omega) & \Sigma_{\alpha\beta}^{*12}(\omega) \\ \Sigma_{\alpha\beta}^{*21}(\omega) & \Sigma_{\alpha\beta}^{*22}(\omega) \end{pmatrix}$$

eigenvalue problem

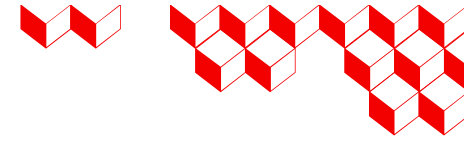
$$\omega_k \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}^k \\ \bar{\mathcal{Z}}^k \end{pmatrix} = \begin{pmatrix} T - \mu \mathbb{I} + \Sigma^{(\infty)11} & \Sigma^{(\infty)12} & \mathcal{C} & \bar{\mathcal{D}}^\dagger \\ \Sigma^{(\infty)21} & -T + \mu \mathbb{I} + \Sigma^{(\infty)22} & \mathcal{D}^T & \bar{\mathcal{C}}^* \\ \mathcal{C}^\dagger & \mathcal{D}^* & \mathcal{E} & \\ \bar{\mathcal{D}} & \bar{\mathcal{C}}^T & -\mathcal{E}^T & \end{pmatrix} \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}^k \\ \bar{\mathcal{Z}}^k \end{pmatrix}$$

Perturbative expansion

$$\begin{aligned} \Sigma_{\alpha\beta}^{*11}(\omega) &= \text{---} \bigcirc \text{---} + \text{---} \bigcirc \text{---} + \text{---} \bigcirc \text{---} + \dots \\ \Sigma_{\alpha\beta}^{*21}(\omega) &= \text{---} \bigcirc \text{---} + \text{---} \bigcirc \text{---} + \text{---} \bigcirc \text{---} + \dots \end{aligned}$$

→ ADC can be generalised to Gorkov scheme

Gorkov ADC



⊙ ADC(n) self-energy expansion

$$\Sigma = \left(\begin{array}{c|c} \text{[Diagram 1]} & \text{[Diagram 2]} \\ \hline \text{[Diagram 3]} & \text{[Diagram 4]} \end{array} \right)$$

$$+ \left(\begin{array}{c|c} \text{[Diagram 5]} + \text{[Diagram 6]} & \text{[Diagram 7]} + \text{[Diagram 8]} \\ \hline \dots & \dots \end{array} \right)$$

$$+ \left(\begin{array}{c|c} \text{[Diagram 9]} + \dots + \text{[Diagram 10]} + \dots & \dots \\ \hline \dots & \dots \end{array} \right)$$

+ ...

ADC(1) \rightarrow HFB

ADC(2) \rightarrow Second-order (uncorrelated 2p1h & 2h1p)

\rightarrow Derived & implemented

[Somà, Duguet, Barbieri 2011, 2014]

ADC(3) \rightarrow Includes Tamm-Dancoff pp, hh, ph ladders (+ more)

\rightarrow Derived

[Barbieri, Duguet, Somà 2022]

ADC(∞)=exact

✗ Missing step: symmetry restoration

○ Observables “contaminated”

○ Effect depends on nucleus and observable

Gorkov ADC



⊙ ADC(n) self-energy expansion

$$\Sigma = \left(\begin{array}{c|c} \text{[diagrams]} & \text{[diagrams]} \\ \hline \text{[diagrams]} & \text{[diagrams]} \end{array} \right) + \left(\begin{array}{c|c} \text{[diagrams]} & \text{[diagrams]} \\ \hline \text{[diagrams]} & \text{[diagrams]} \end{array} \right) + \left(\begin{array}{c|c} \text{[diagrams]} & \text{[diagrams]} \\ \hline \text{[diagrams]} & \text{[diagrams]} \end{array} \right) + \dots$$

ADC(1)

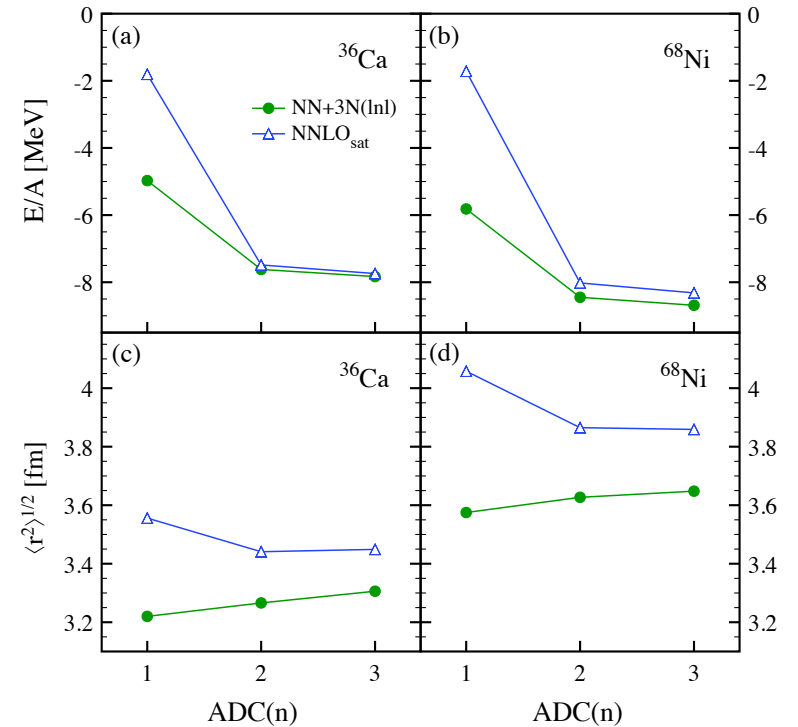
ADC(2)

ADC(3)

ADC(∞)=exact

ADC(n) convergence

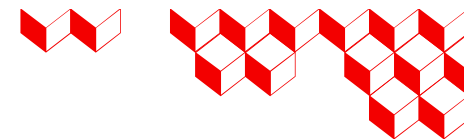
[Somà *et al.*, 2020]



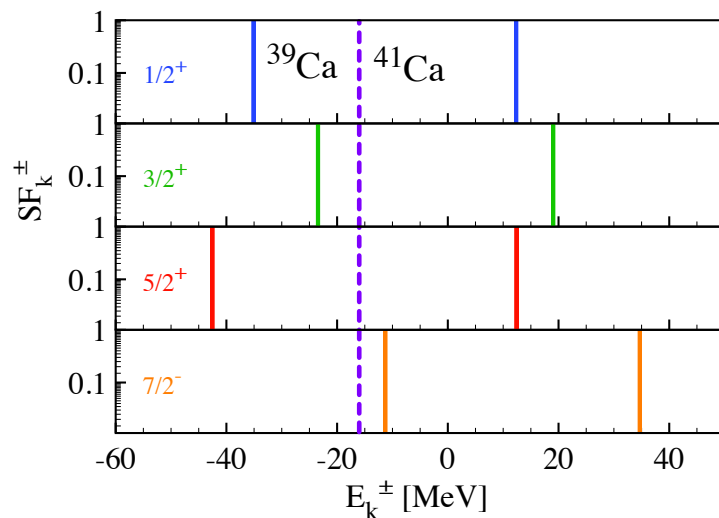
✗ Missing step: symmetry restoration

- Observables “contaminated”
- Effect depends on nucleus and observable

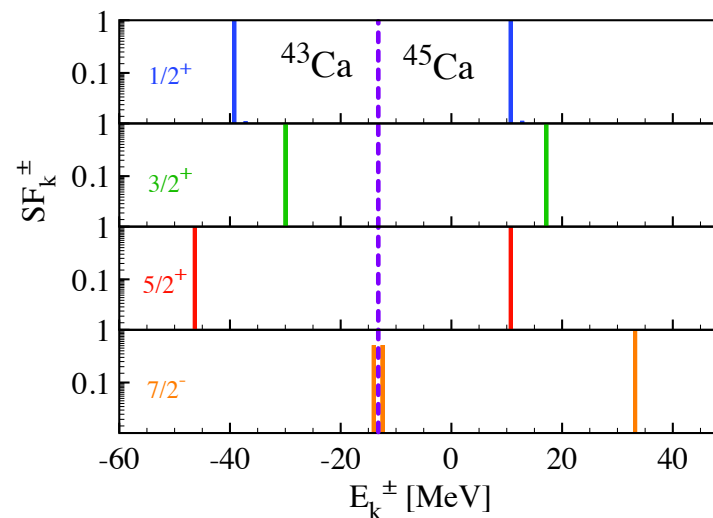
Gorkov ADC



Dyson
ADC(1)



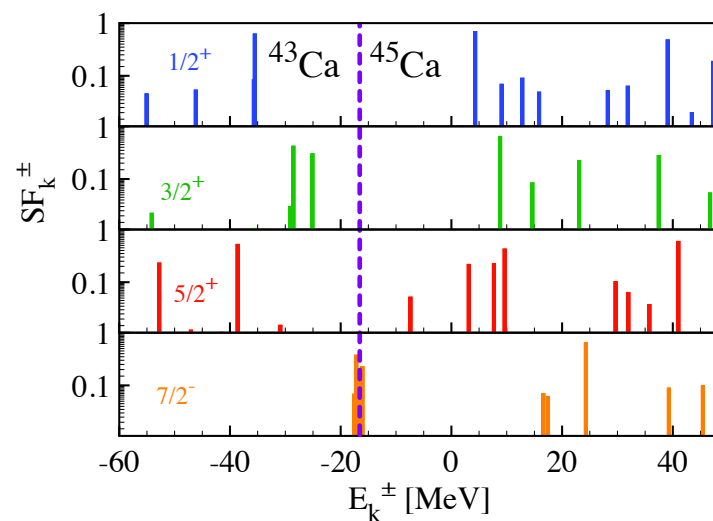
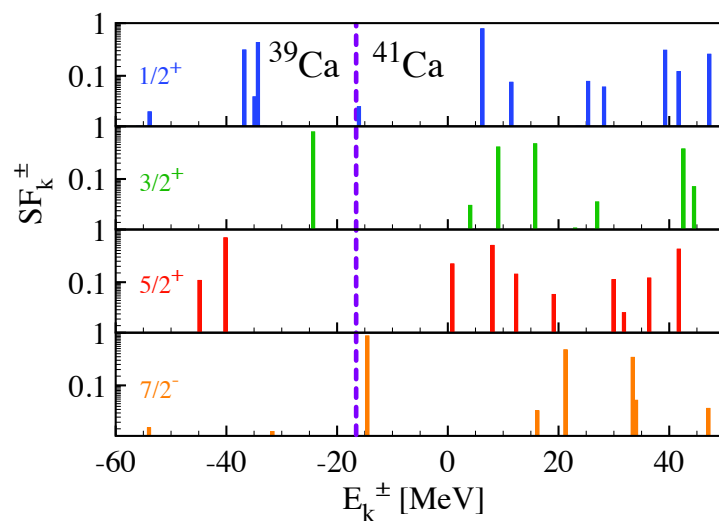
Static pairing
→



Gorkov
ADC(1)

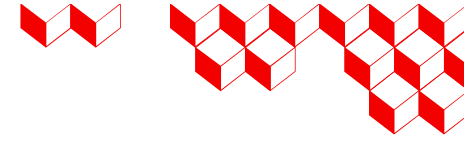
Dynamical
fluctuations
↓

Dyson
ADC(2)



Gorkov
ADC(2)

Binding energies



Systematic calculations around semi-magic calcium chain

- Gorkov ADC(2) scheme
- Hamiltonians: $\text{NN}+3\text{N}(\text{lnl})$ & NNLO_{sat}
 - $\text{NN}+3\text{N}(\text{lnl})$ energies
 - NNLO_{sat} radii
- All even-even isotopes with $18 \leq Z \leq 24$ & $14 \leq N \leq 40$
 - Energies of odd-even neighbours for free

Eur. Phys. J. A (2021) 57:135
<https://doi.org/10.1140/epja/s10050-021-00437-4>

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Regular Article - Theoretical Physics

Moving away from singly-magic nuclei with Gorkov Green's function theory

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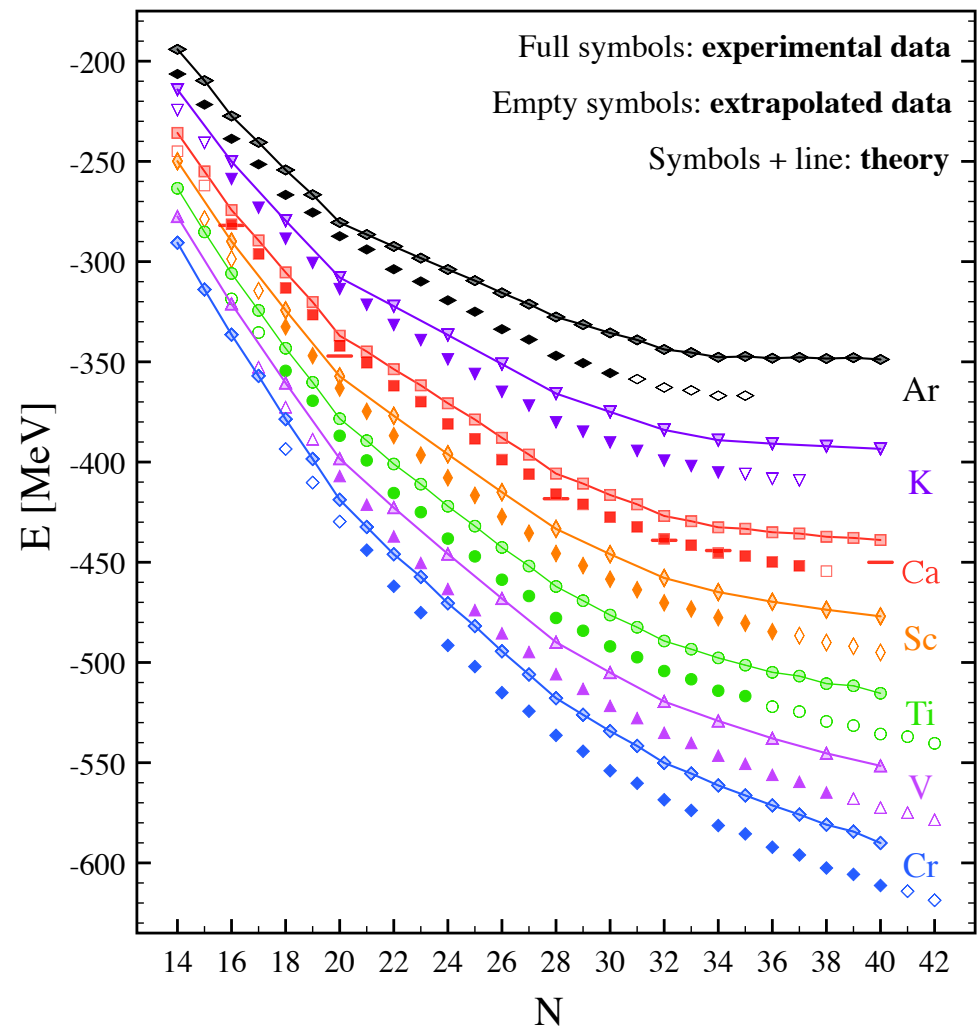
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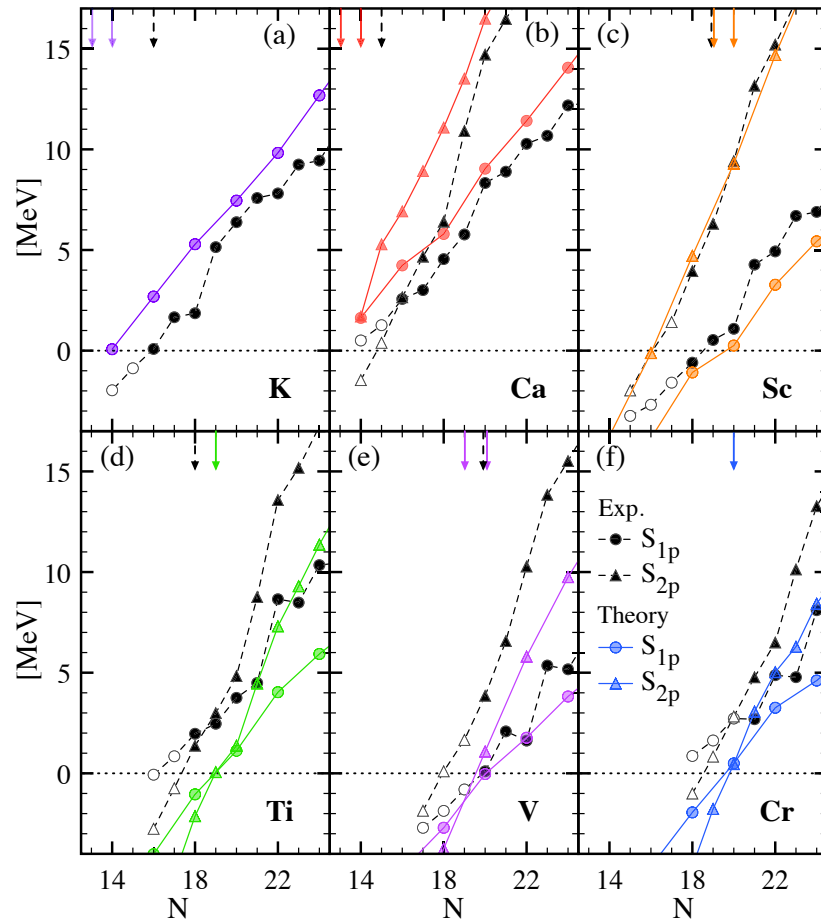
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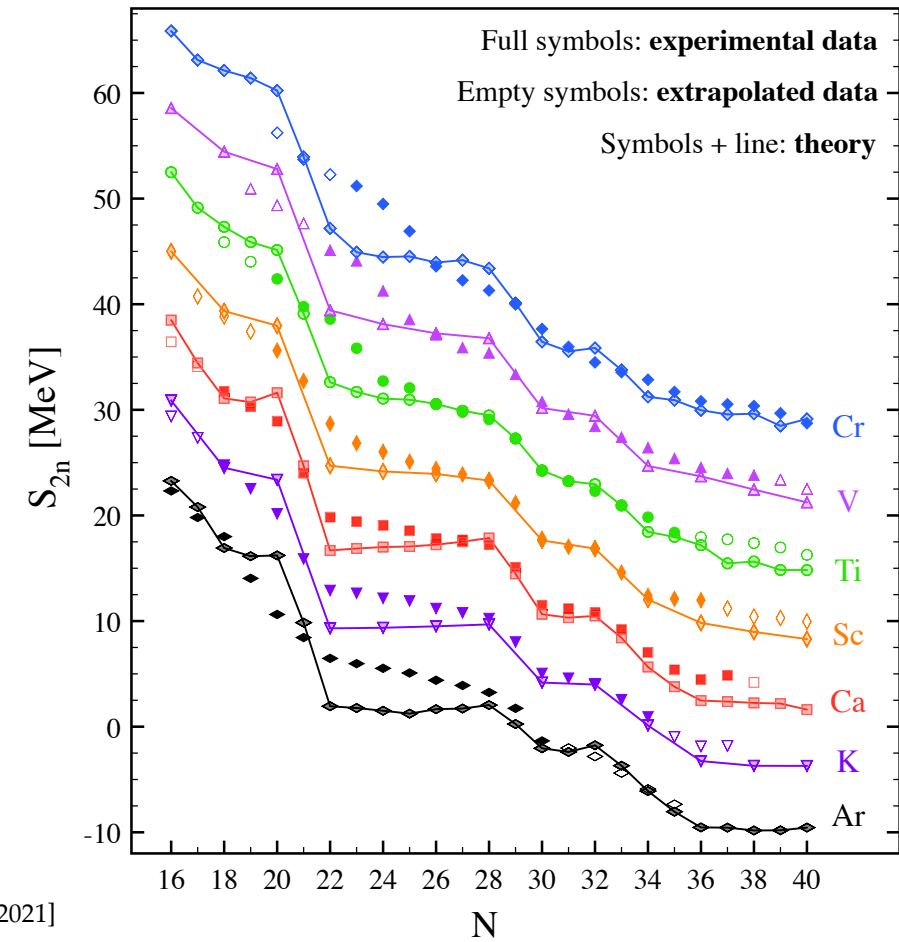
Separation energies



One- & two-proton separation energies

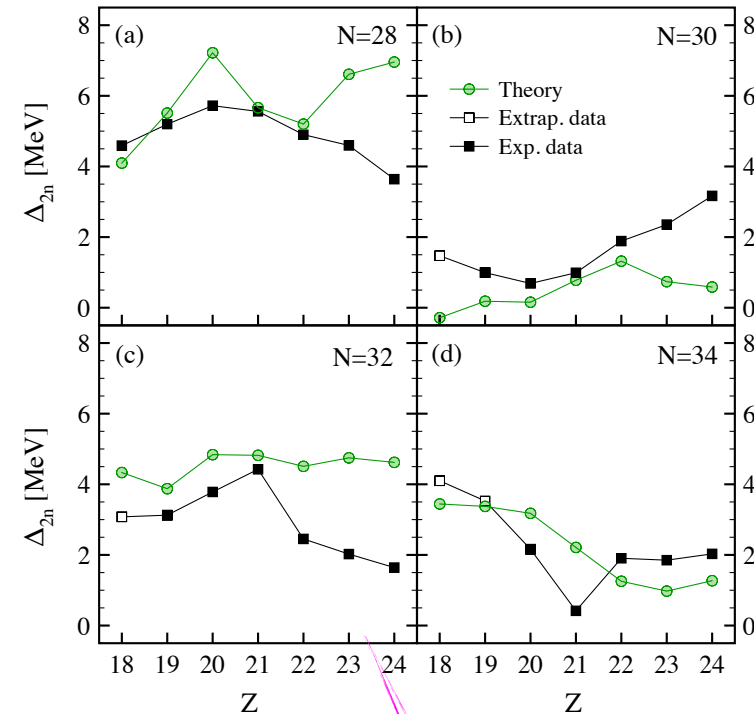
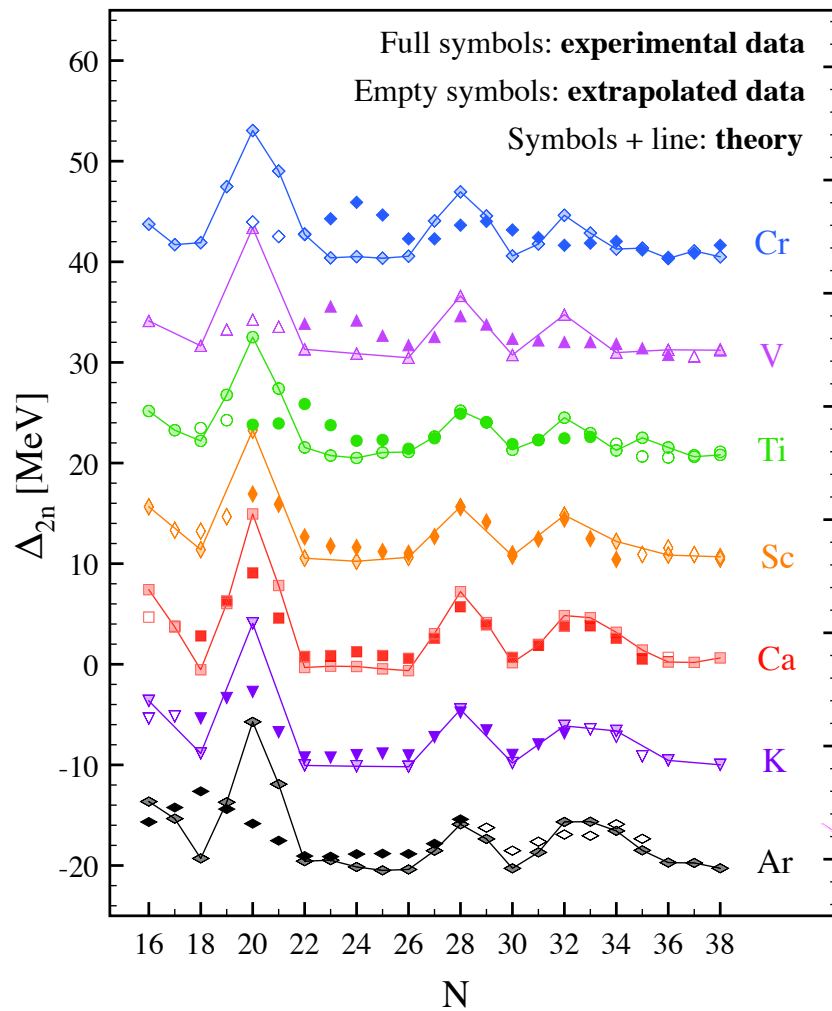


Two-neutron separation energies



[Somà *et al.*, 2021]

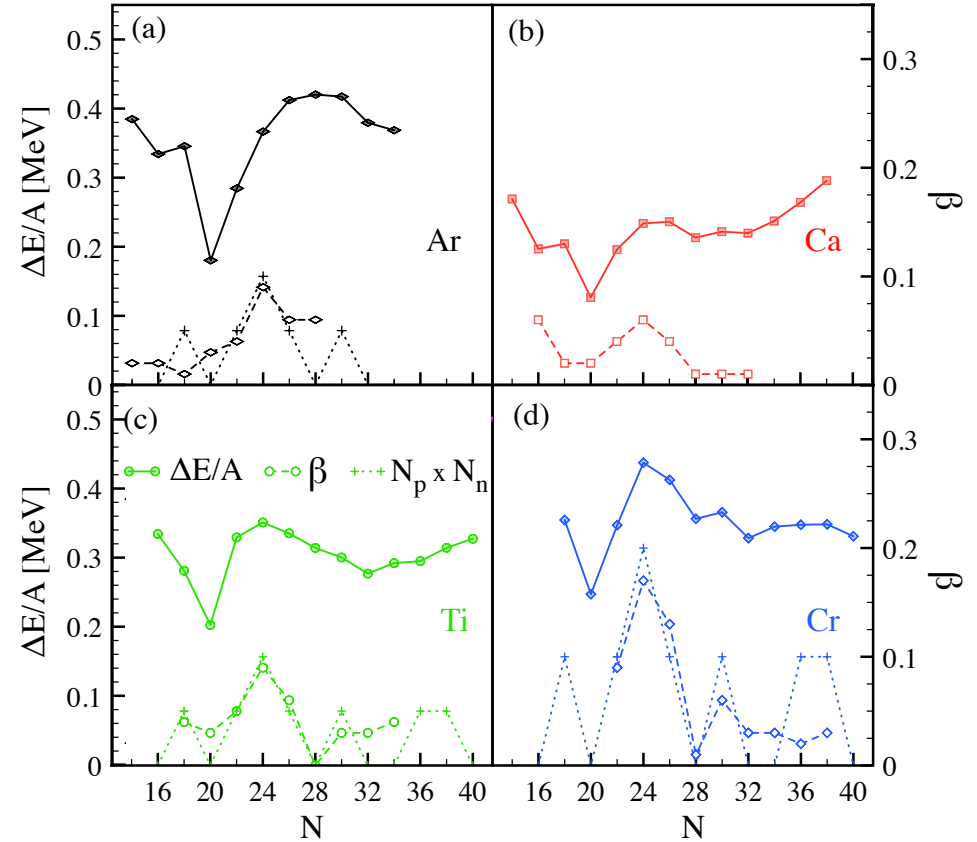
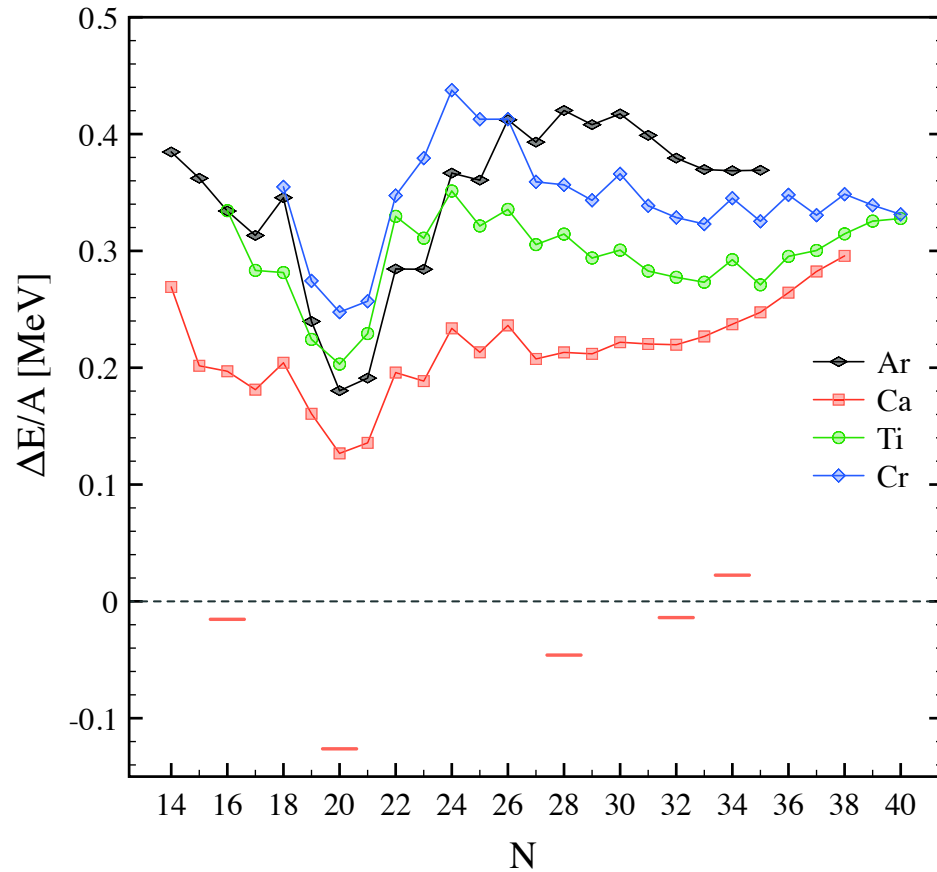
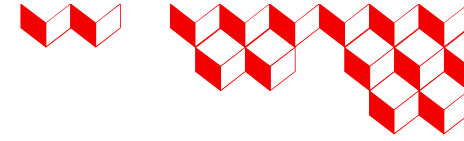
Two-neutron gaps



Evolution with Z (roughly) captured

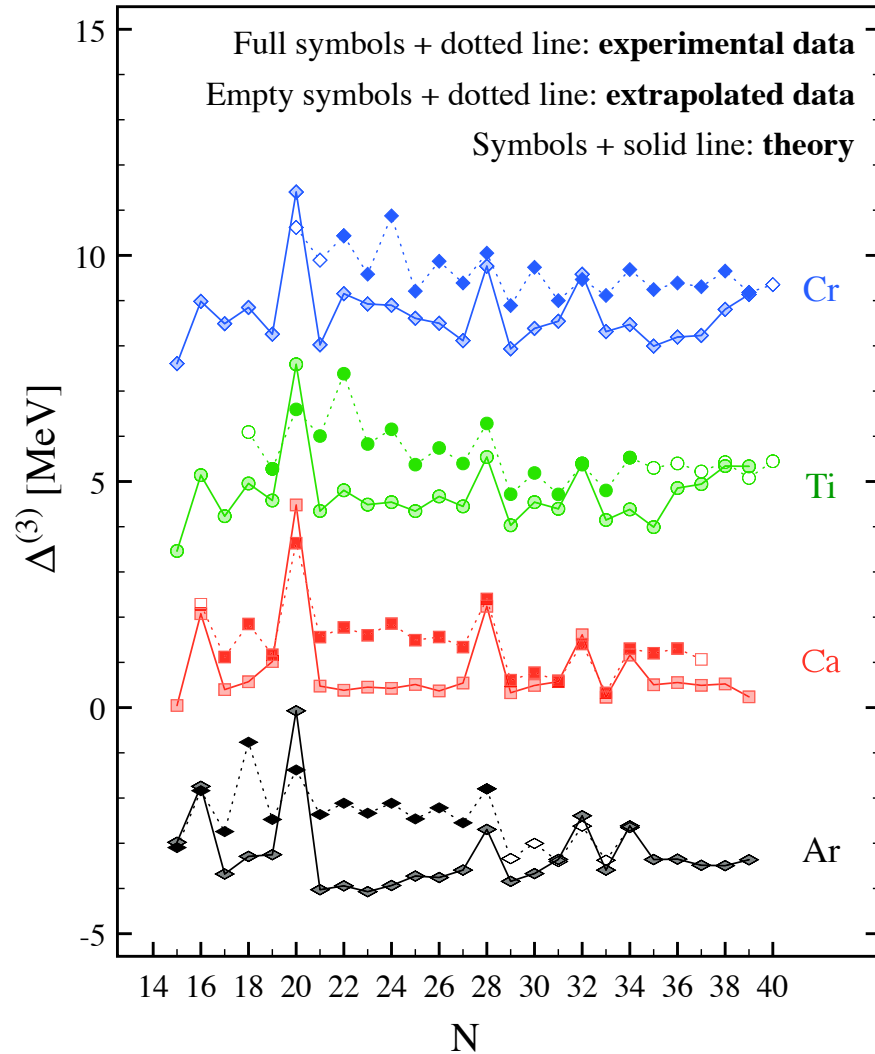
Magic number emerge "ab initio"

Fingerprint of deformation



- Differences with experiment shows trends that seem to **correlate with deformation**
- Supported by simple estimate of β [Dobaczewski *et al.*, 1988] and multi-reference EDF calculations [Bender *et al.*, 2006]

Three-point mass differences

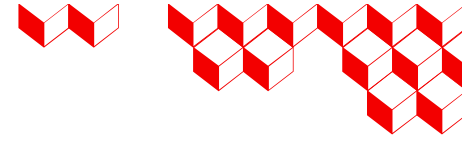


- **Gaps too small** (even smaller than at HFB level)
 - Anti-pairing effect of fragmentation
 - Insufficient increase in m^* ?
 - Effective pairing interaction not sufficiently attractive?

→ **Coupling to collective excitations necessary?**
(cf. Vigezzi & Barranco)

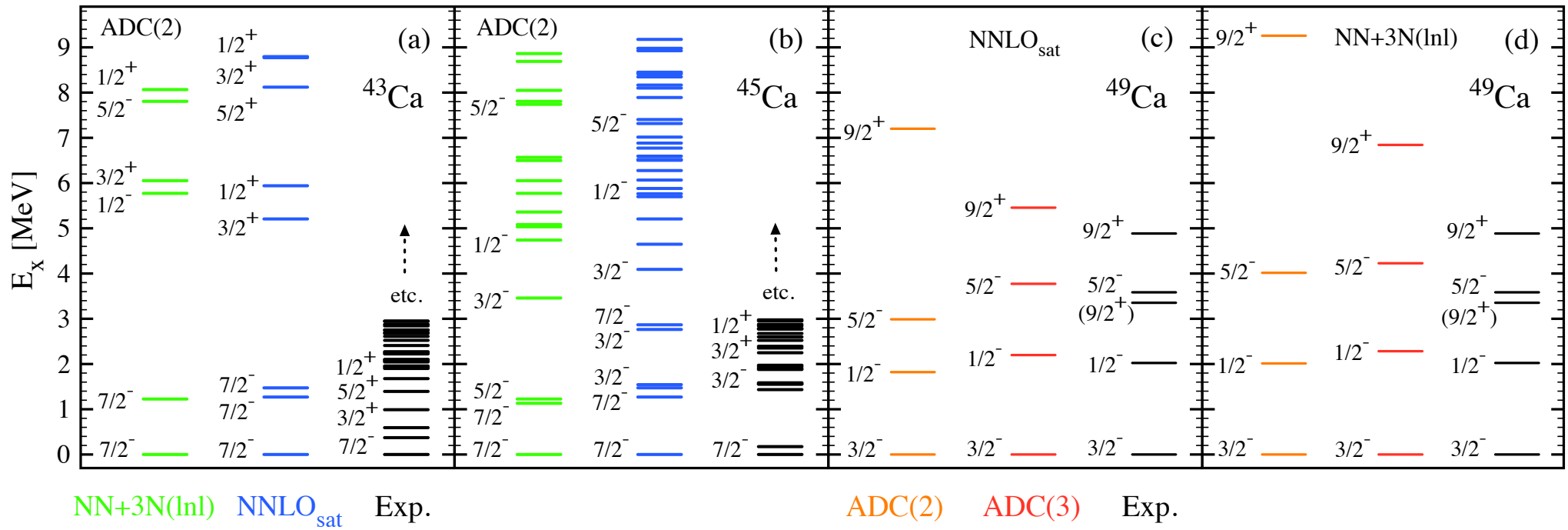
- Results consistent **across isotopic chains**
- **Effect of particle-number projection?**
 - Signatures in other observables?

Spectra (neutrons)



One-body propagator gives access to one-nucleon removal/addition spectra

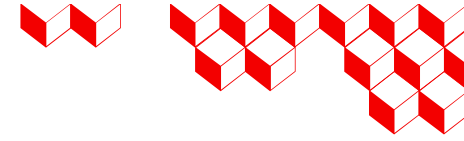
Neutron removal/addition from ^{44}Ca and ^{48}Ca



One-neutron addition from closed-shell ^{48}Ca shows good agreement with data

Spectra from open-shell ^{48}Ca display significantly lower density of states → Another signature of **too low effective mass**

Spectra (protons)

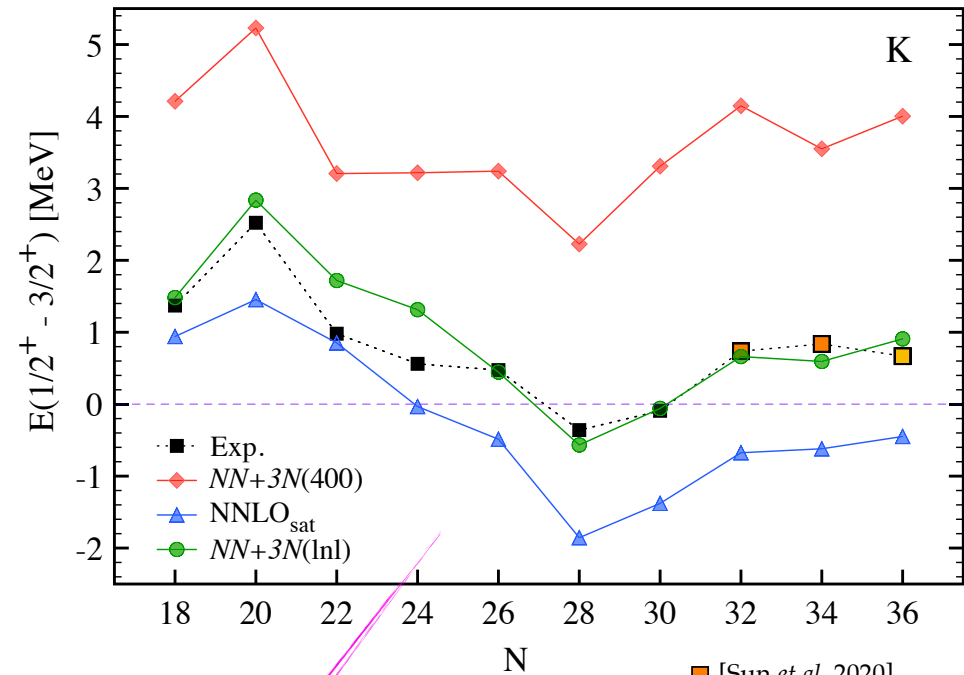
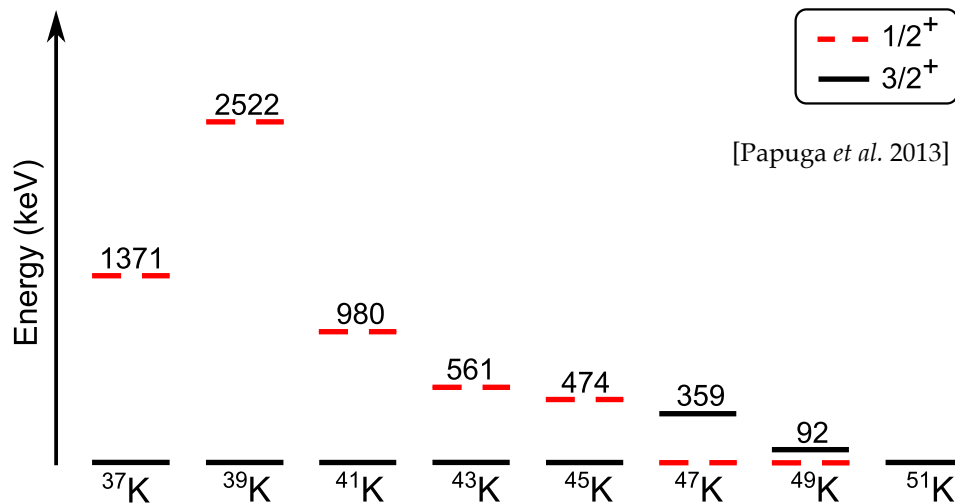


◉ Situation qualitatively different for closed-shell species along the isotopic chain

◉ Application to K isotopes → **inversion & re-inversion of g.s. spin**

[Somà *et al.* 2020]

Laser spectroscopy COLLAPS @ ISOLDE

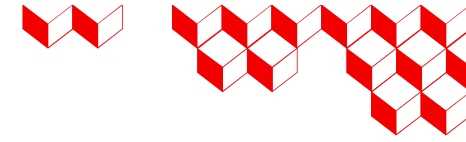


■ [Sun *et al.* 2020]

■ [Koiwai *et al.* 2022]

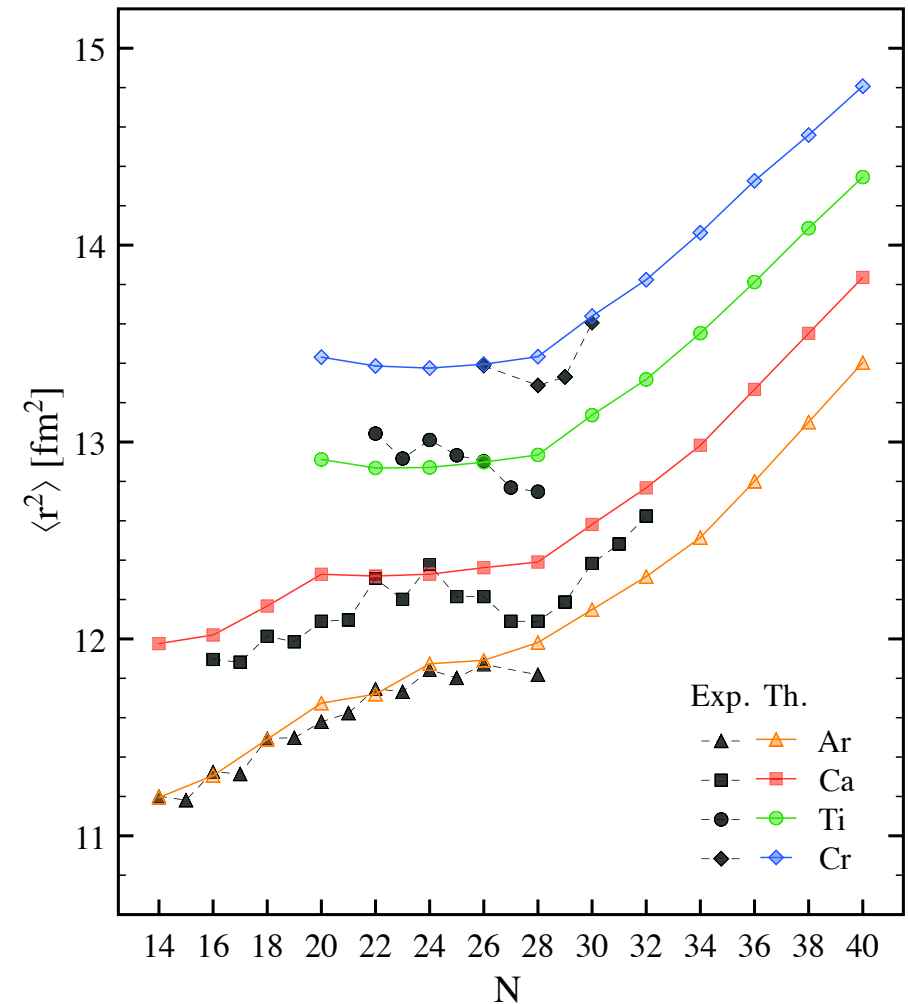
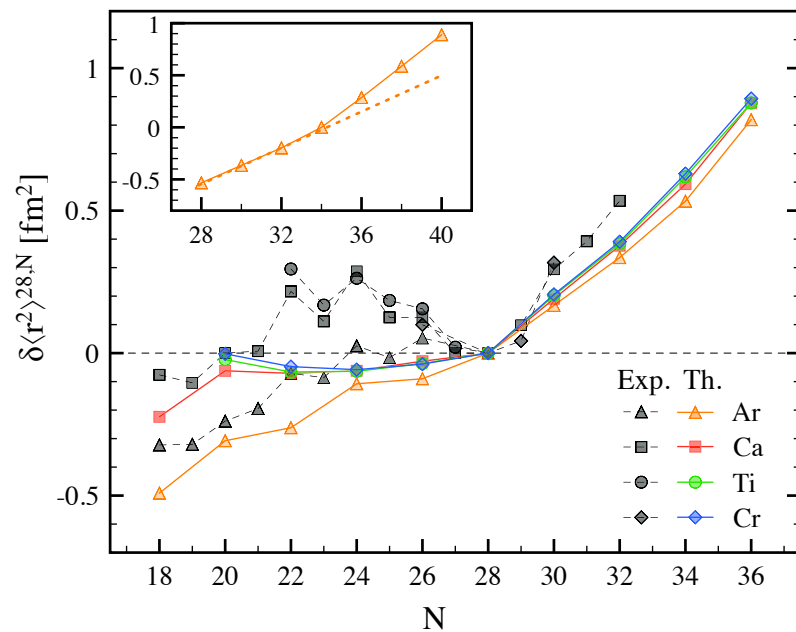
Evolution of g.s.-excited state difference nicely captured

Charge radii

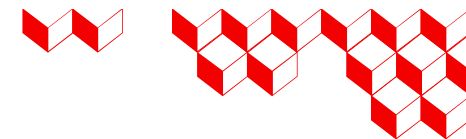


◉ Charge radii can be evaluated **along even-Z chains**

- ◉ NNLO_{sat} delivers nuclei of the right size
- ◉ **Some exp. features reproduced, but not all**
 - ✓ Change of slope as Z decreases captured
 - ✗ Parabolic behaviour between N=20 and N=28 absent
 - ✗ Kink at N=28 underestimated



Deformed SCGF



◉ Breaking rotational invariance → Description of **doubly open-shell nuclei**

◉ Dyson m -scheme

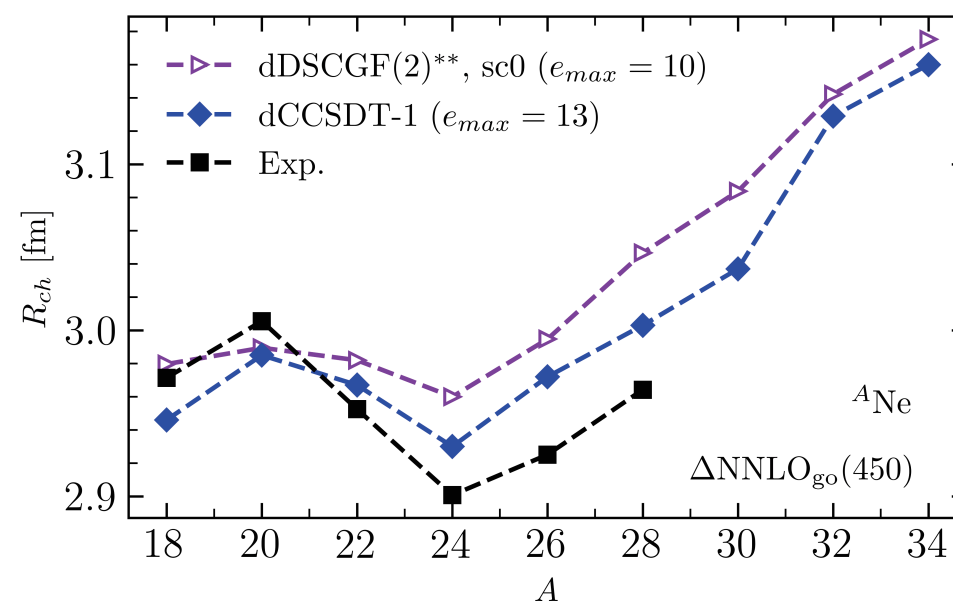
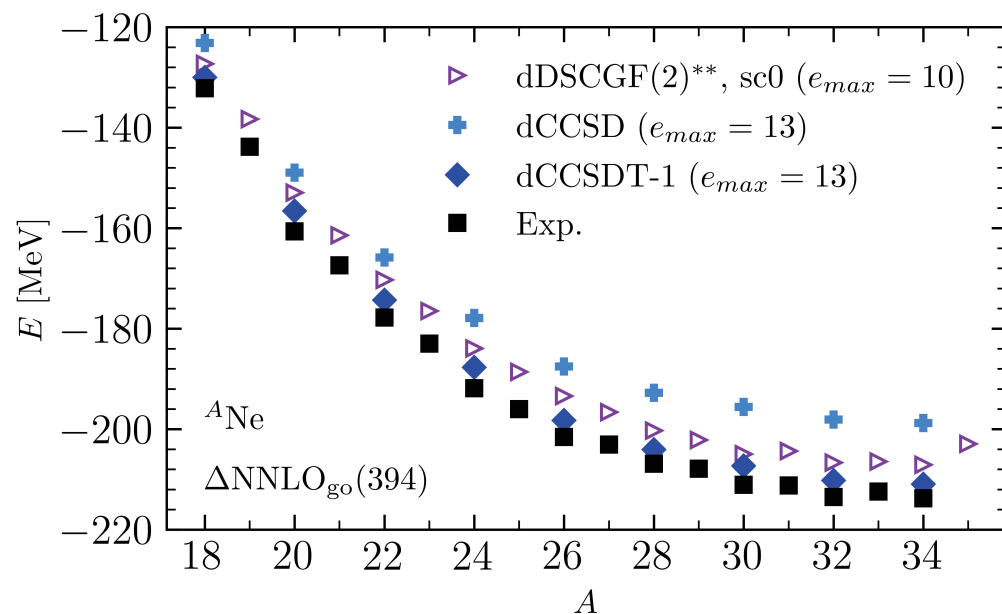
◉ **ADC(2)** implemented

◉ All following results still

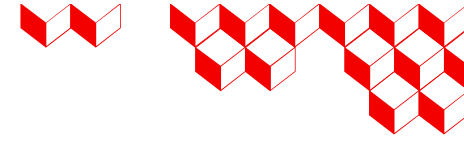
Preliminary

[Scalei, PhD Thesis 2024 & Scalei *et al.* in preparation]

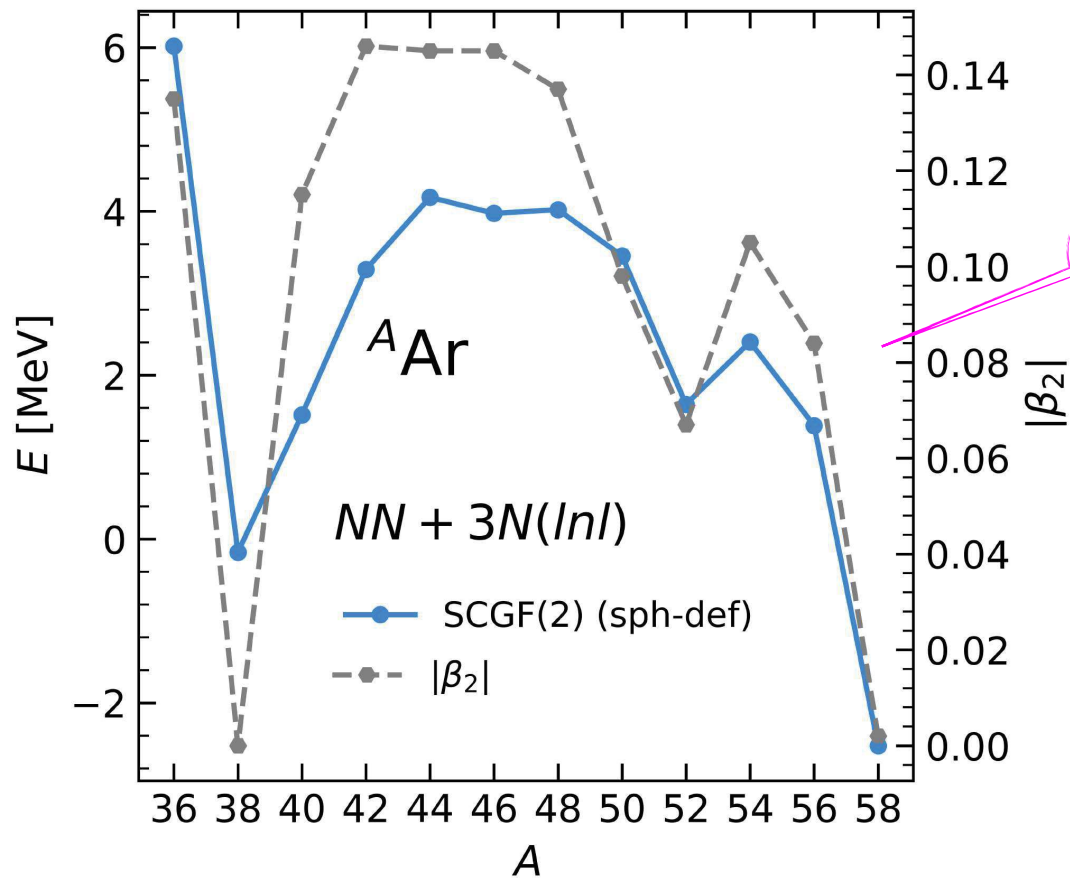
◉ Benchmark against CCSD & CCSDT-1 calculations



Fingerprint of deformation (part II)



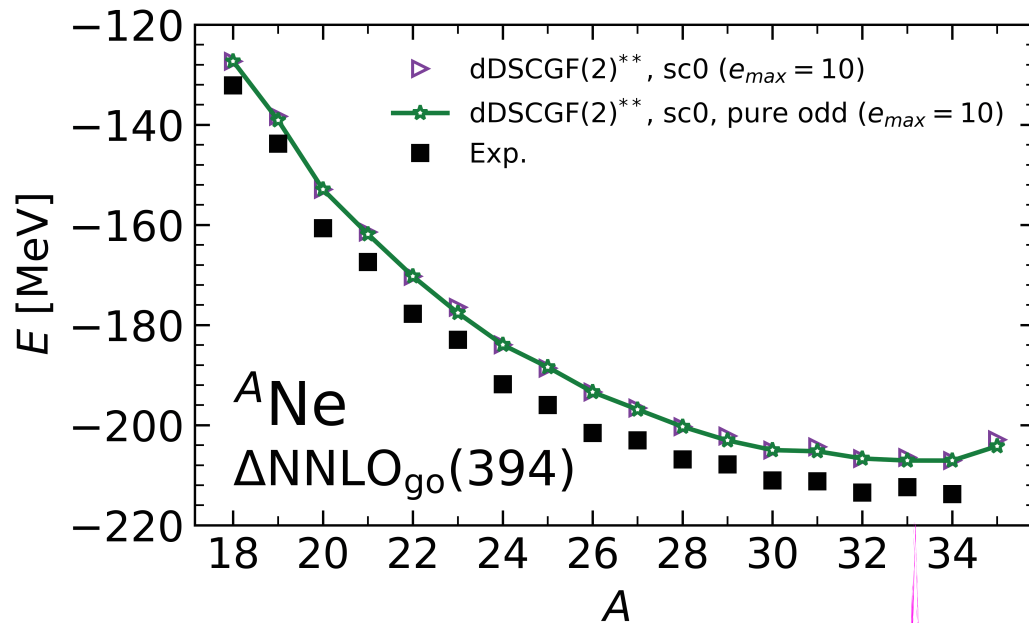
- Comparison with spherical Gorkov SCGF highlights **effects of deformation on binding energies**
- Argon isotopes display **oblate** g.s. deformations



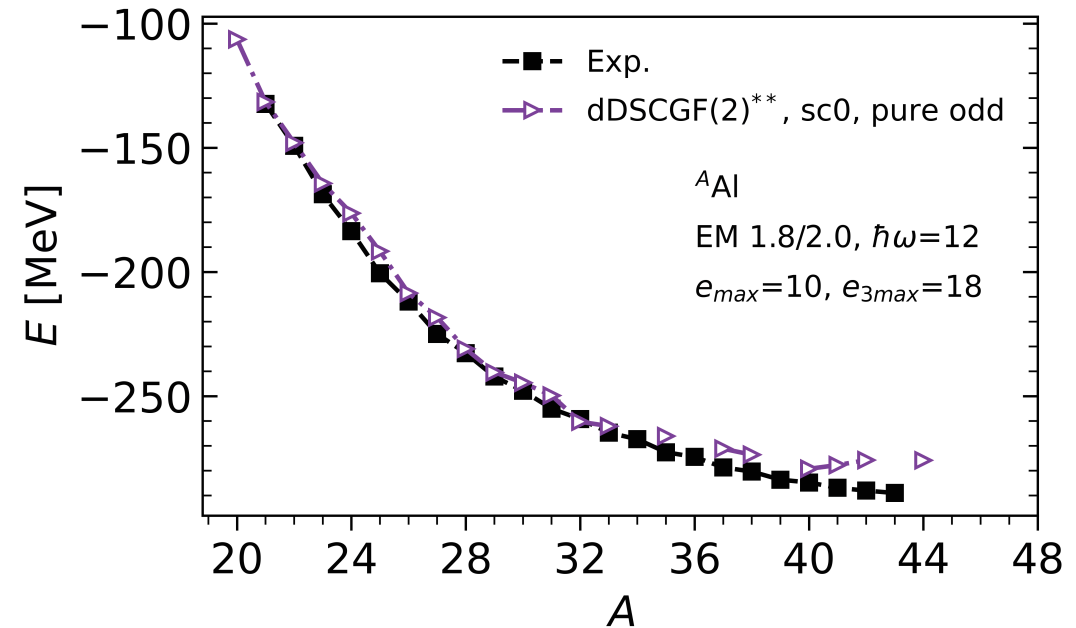
Difference shows clear correlation with deformation

Odd systems

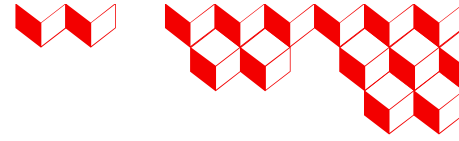
- ◉ Necessity of working in m -scheme opens up the possibility of targeting ground states with $J \neq 0 \rightarrow$ **odd nuclei**
- ◉ Consistency of past approximations can be directly tested
- ◉ Description of **full odd-Z chains** becomes available (i.e. both odd-even and odd-odd isotopes)



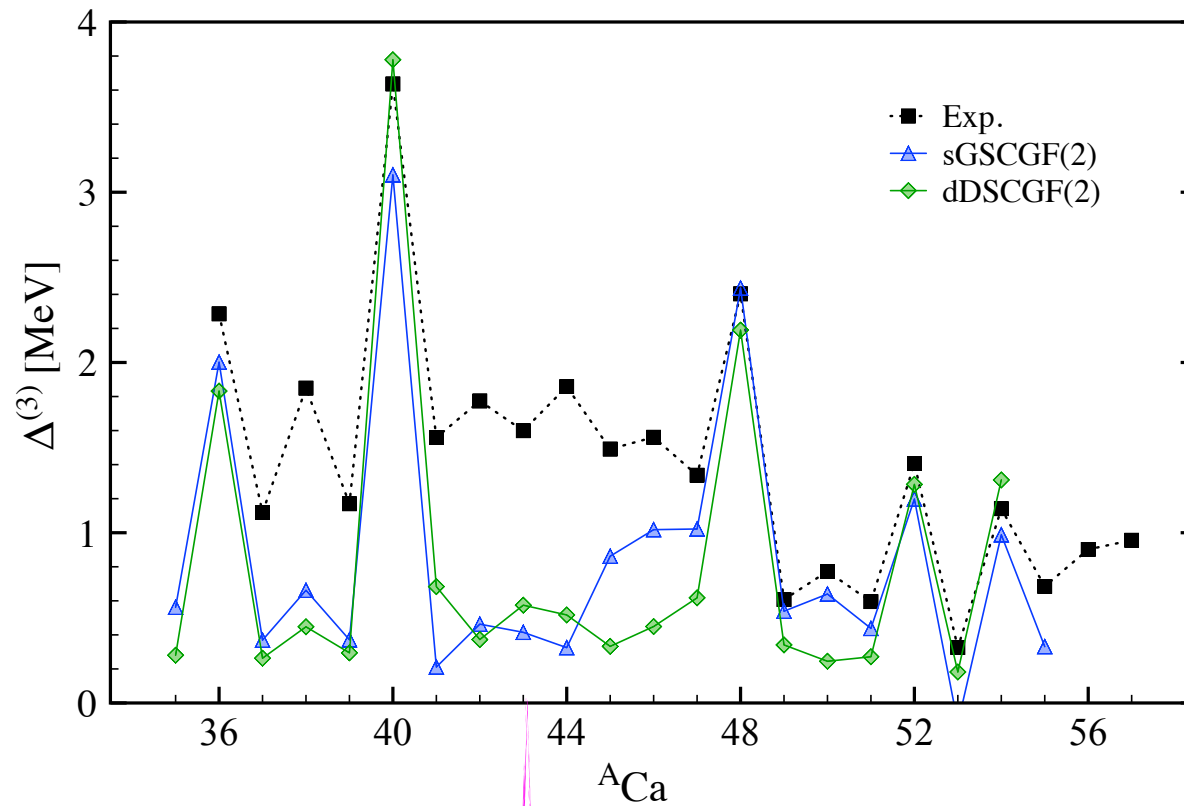
Direct & “from-even” calculations give very consistent results



Three-point mass differences (part II)

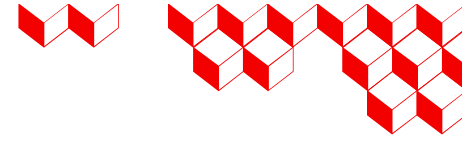


- What is the resulting behaviour on three-point mass difference?



Very similar $\Delta^{(3)}$ when **breaking U(1) or SU(2) at the ADC(2) level**

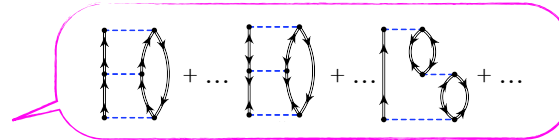
Beyond Gorkov-ADC(2)



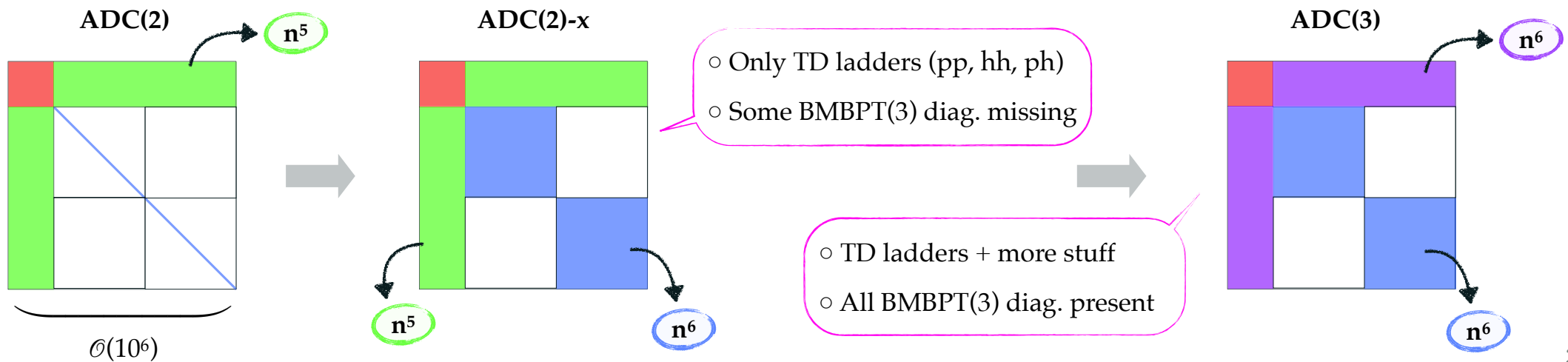
◎ “Can you make it LOUDER?” [© G. Hagen]

○ ADC(3) introduces couplings to **collective fluctuations**

○ ADC(2) → ADC(3): same matrix form and dimensions, but cost of computation significantly increases



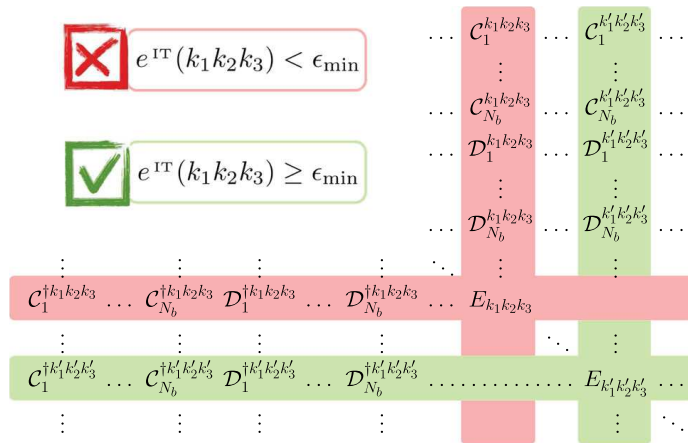
$$\omega_k \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}^k \\ \bar{\mathcal{Z}}^k \end{pmatrix} = \begin{pmatrix} T - \mu \mathbb{I} + \Sigma^{(\infty)11} & \Sigma^{(\infty)12} & \mathcal{C} & \bar{\mathcal{D}}^\dagger \\ \Sigma^{(\infty)21} & -T + \mu \mathbb{I} + \Sigma^{(\infty)22} & \mathcal{D}^T & \bar{\mathcal{C}}^* \\ \mathcal{C}^\dagger & \mathcal{D}^* & \mathcal{E} & \\ \bar{\mathcal{D}} & \bar{\mathcal{C}}^T & -\mathcal{E}^T & \end{pmatrix} \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}^k \\ \bar{\mathcal{Z}}^k \end{pmatrix}$$



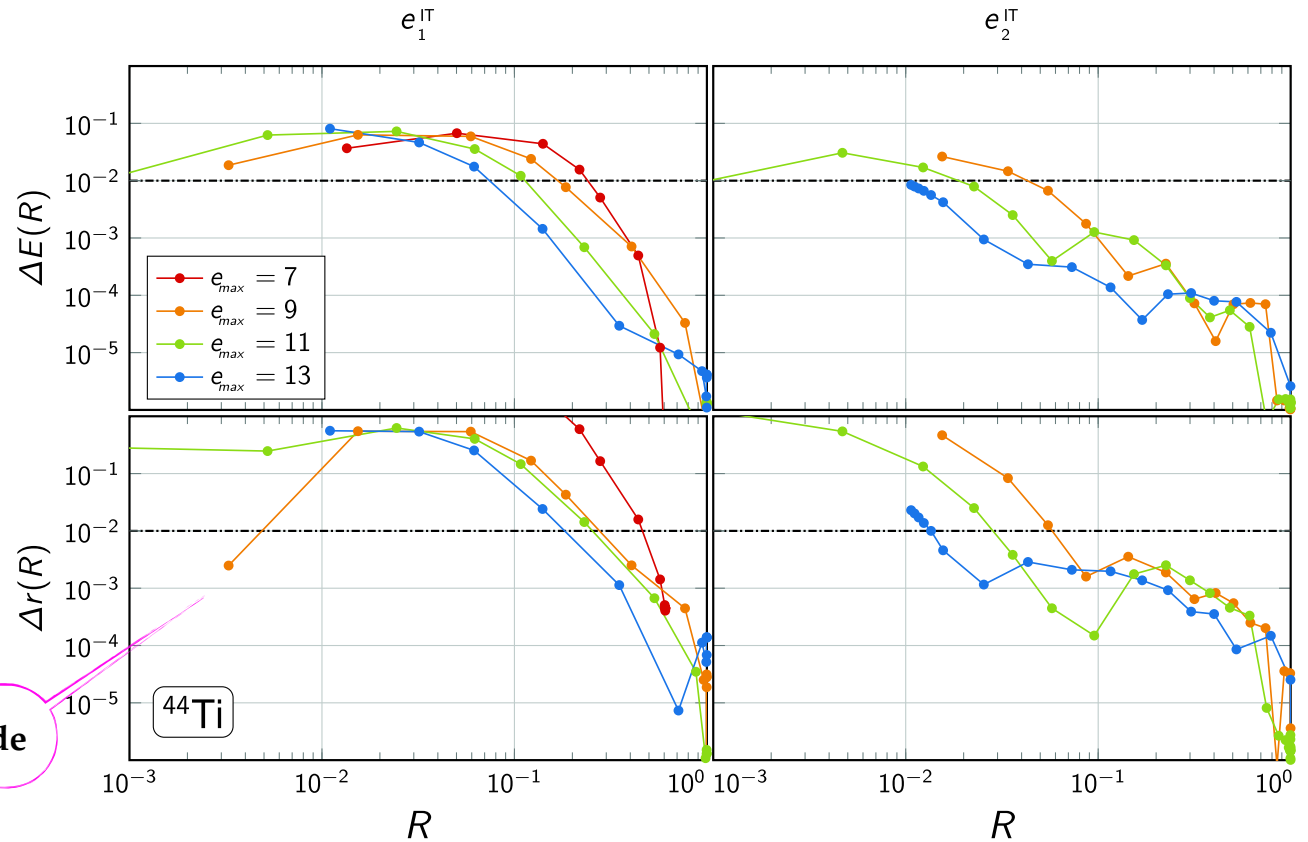
Importance truncation

- ◉ **Idea:** discard entries (in the Gorkov matrix) that contribute little
 - ◉ Two IT measures $\rightarrow \mathbf{e}_1$ (based on amplitudes only) & \mathbf{e}_2 (based on BMBPT energy)
 - ◉ Analyse error of total energies & radii as a function of the IT truncation

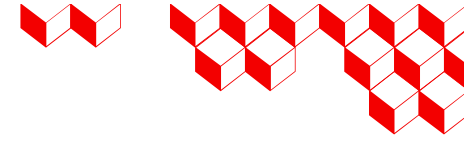
[Porro *et al.* 2021]



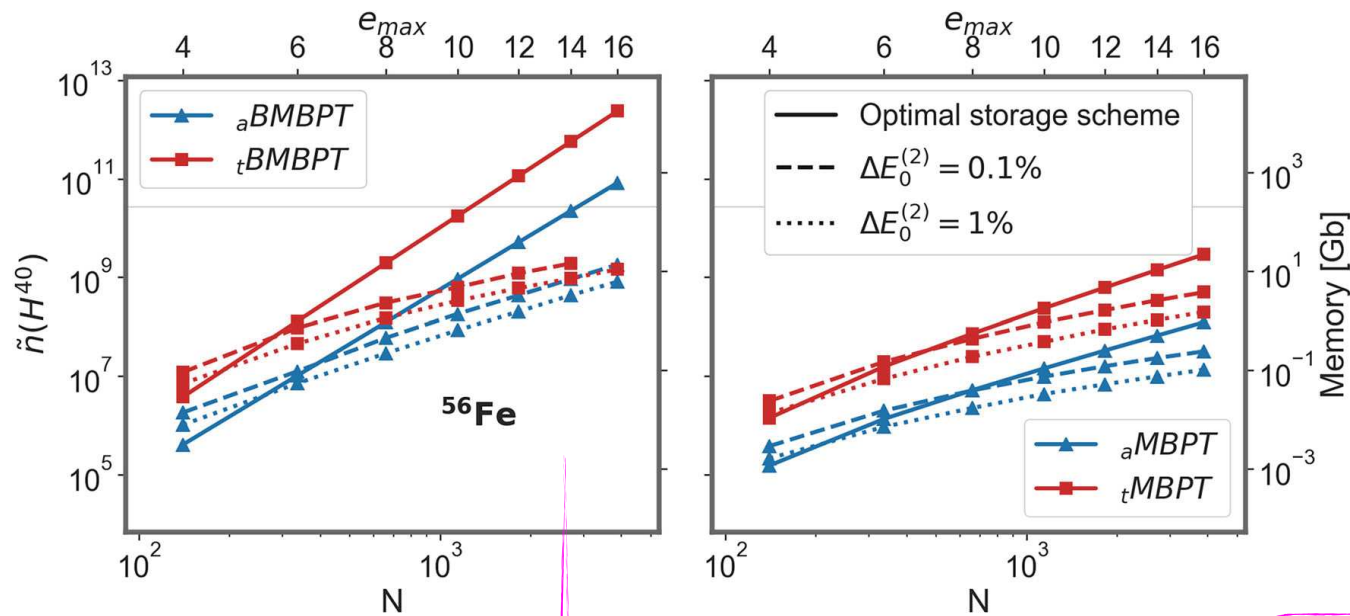
Dimensions can be reduced by 2 orders of magnitude



Tensor factorisation

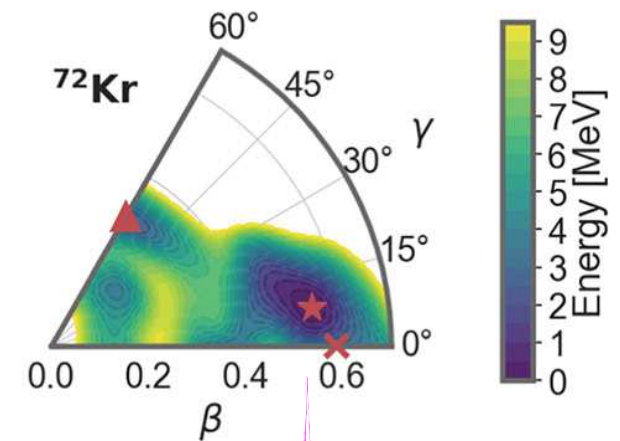


- ◉ **Idea:** use **factorised forms of many-body tensors** to reduce memory & computational costs
 - Randomised singular value decomposition (rSVD) → Does not require calculation of full tensors
 - Applications to axial & triaxial (B)MBPT



Gain becomes significant for **large bases** → Promising for heavy nuclei

[Frosini, Duguet, Tamagno 2024]



E.g.: triaxial calculation of ^{72}Kr **previously undoable**

Conclusions



◉ Gorkov ADC(2)

- Good reproduction of energies & low-lying spectra
- Reasonable reproduction of radii (& densities)
- Pairing too weak (← Three-point mass differences, spectra at mid-shell)

◉ Deformed ADC(2)

- Successful benchmarks, promising results
- Allows direct computation of odd-even & odd-odd systems
- Symmetry restoration even more needed than for particle-number breaking (e.g., spectra)

◉ Towards Gorkov ADC(3)

- Formalism derived
- Implementation require careful optimisation & use of dimensionality-reduction techniques

Thanks to

T. Duguet,
C. Barbieri,
A. Porro,
P. Navrátil

A. Scalesi
T. Duguet,
M. Frosini