Green's function studies from oxygen to nickel

- **Beyond energy systematics: charge & matter radii in oxygen**

  V. Lapoux, VS, C. Barbieri, H. Hergert, J. D. Holt, S. R. Stroberg (to be submitted)

- **Testing the performance of chiral interactions in medium-mass nuclei**

  VS, C. Barbieri, T. Duguet, P. Navrátil (in preparation)

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Set-up

⊙ **Two sets of 2N+3N chiral interactions**

➟ Conventional* N^3LO 2N (500 MeV) + N^3LO 3N (400 MeV) [**EM**]

✓ SRG-evolved to 1.88-2.0 fm^{-1} [Entem & Machleidt 2003; Navrátil 2007; Roth *et al*. 2012]

➟ Unconventional* N^2LO 2N+3N (450 MeV) [**$NNLO_{sat}$**] [Ekström *et al*. 2015]

✓ bare

* *With respect to the usual reductionist strategy of ab initio calculations*

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EM

○ LECs fitted on A=2, 3, 4

○ **Sequential** optimisation

$NNLO_{sat}$

○ LECs fitted on $A\leq25$

○ **Simultaneous** optimisation

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  * *With respect to the usual reductionist strategy of ab initio calculations*

- **Different many-body approaches**

  - ➟ Self-consistent Green's functions
    - ○ *Closed-shell Dyson scheme* [**DGF**] [Schirmer *et al*. 1983; Cipollone, Barbieri & Navrátil 2013; …]
    - ○ *Open-shell Gorkov scheme* [**GGF**] [Somà, Duguet & Barbieri 2011, …]

  - ➟ In-medium similarity renormalisation group
    - ○ *Closed-shell single-reference scheme* [**SR-IMSRG**] [Tsukiyama, Bogner & Schwenk 2011, …]
    - ○ *Open-shell multi-reference scheme* [**MR-IMSRG**] [Hergert *et al*. 2013, …]

Self-consistent Green's function theory

- All nucleons active, polynomial scaling (cf. CC and IMSRG)
- Self-energy expansion follows Algebraic Diagrammatic Construction (ADC)
- Gorkov scheme: **use symmetry breaking** (particle number) **to account for pairing**

Dyson/Gorkov equation

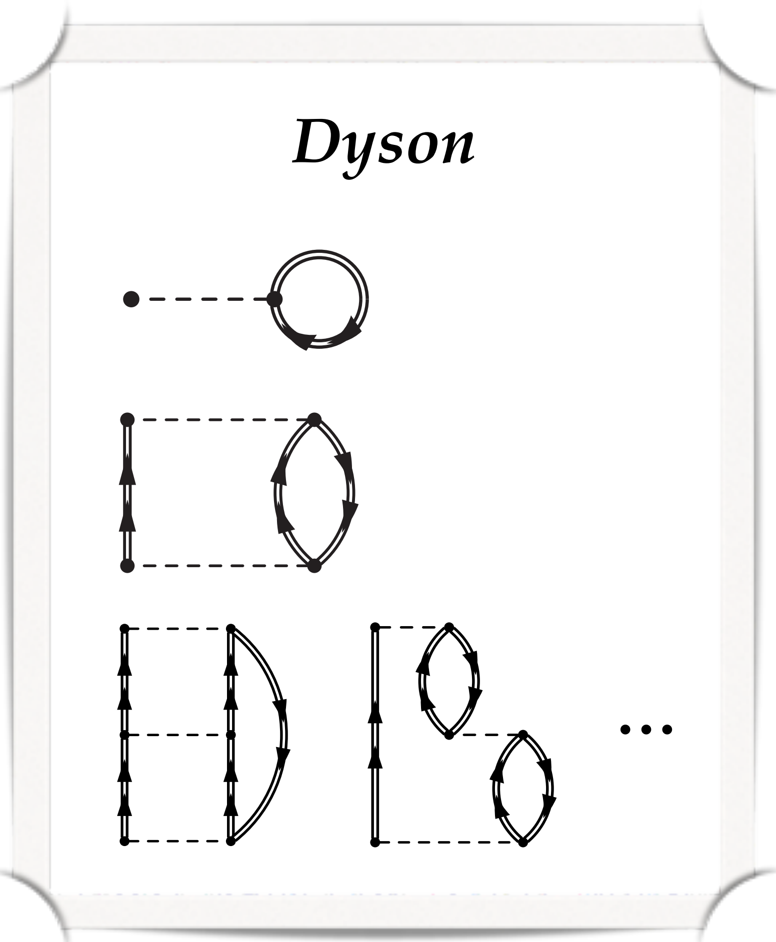
$$\mathbf{G}_{ab}(\omega) = \mathbf{G}^{(0)}_{ab}(\omega) + \sum_{cd} \mathbf{G}^{(0)}_{ac}(\omega)\, \mathbf{\Sigma}^{\star}_{cd}(\omega)\, \mathbf{G}_{db}(\omega)$$

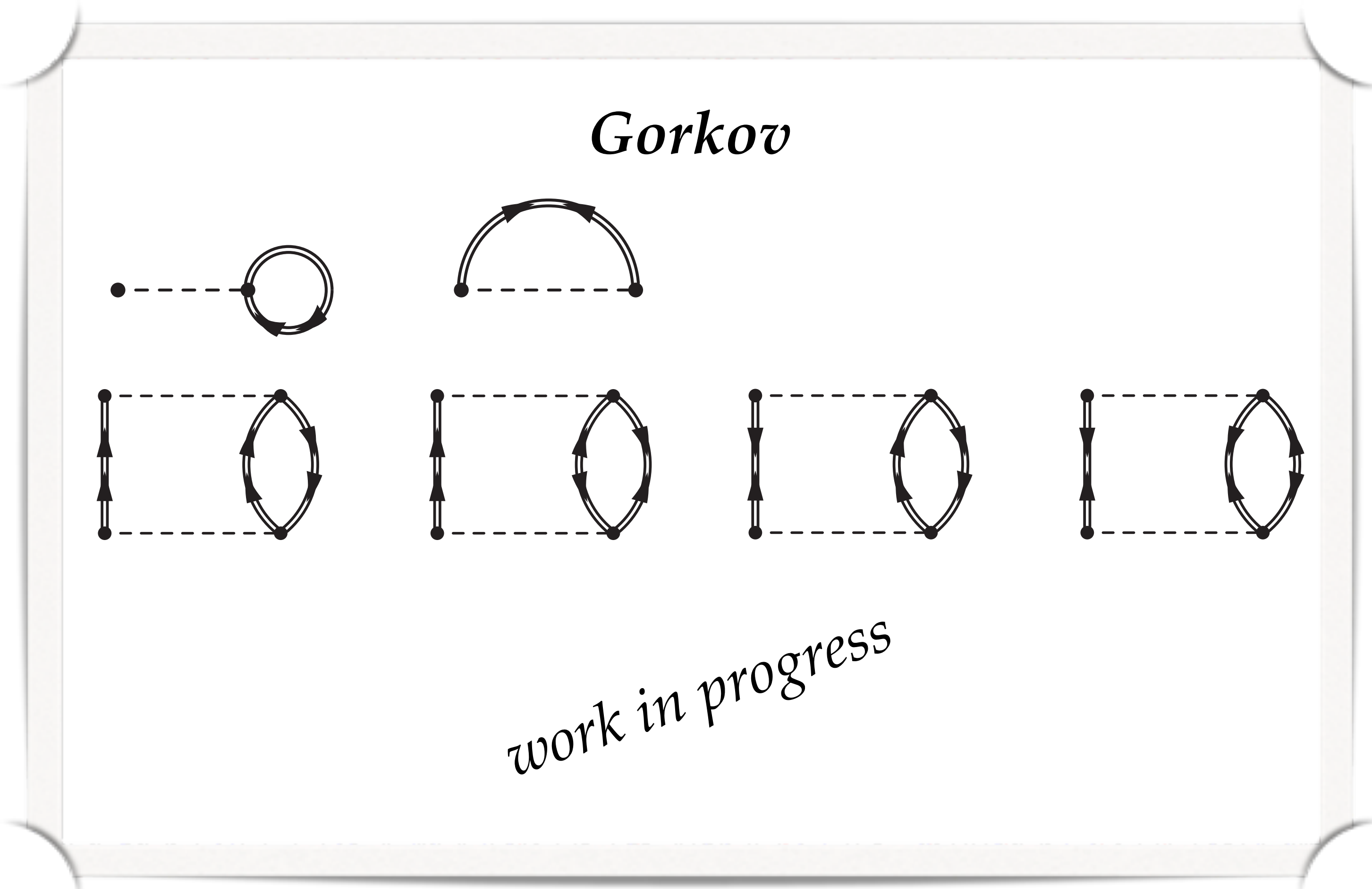
with $\mathbf{G}(\omega) = \begin{pmatrix} G^{11}(\omega) & G^{12}(\omega) \\ G^{21}(\omega) & G^{22}(\omega) \end{pmatrix}$

ADC(1)

ADC(2)

ADC(3)





Self-consistent Green's function theory

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with

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

$$G^{12}_{ab}(\omega) = \sum_k \left\{ \frac{\mathcal{U}^k_a \mathcal{V}^{k*}_b}{\omega - \omega_k + \mathrm{i}\eta} + \frac{\bar{\mathcal{V}}^{k*}_a \bar{\mathcal{U}}^k_b}{\omega + \omega_k - \mathrm{i}\eta} \right\}$$

Energy *dependent* eigenvalue problem

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

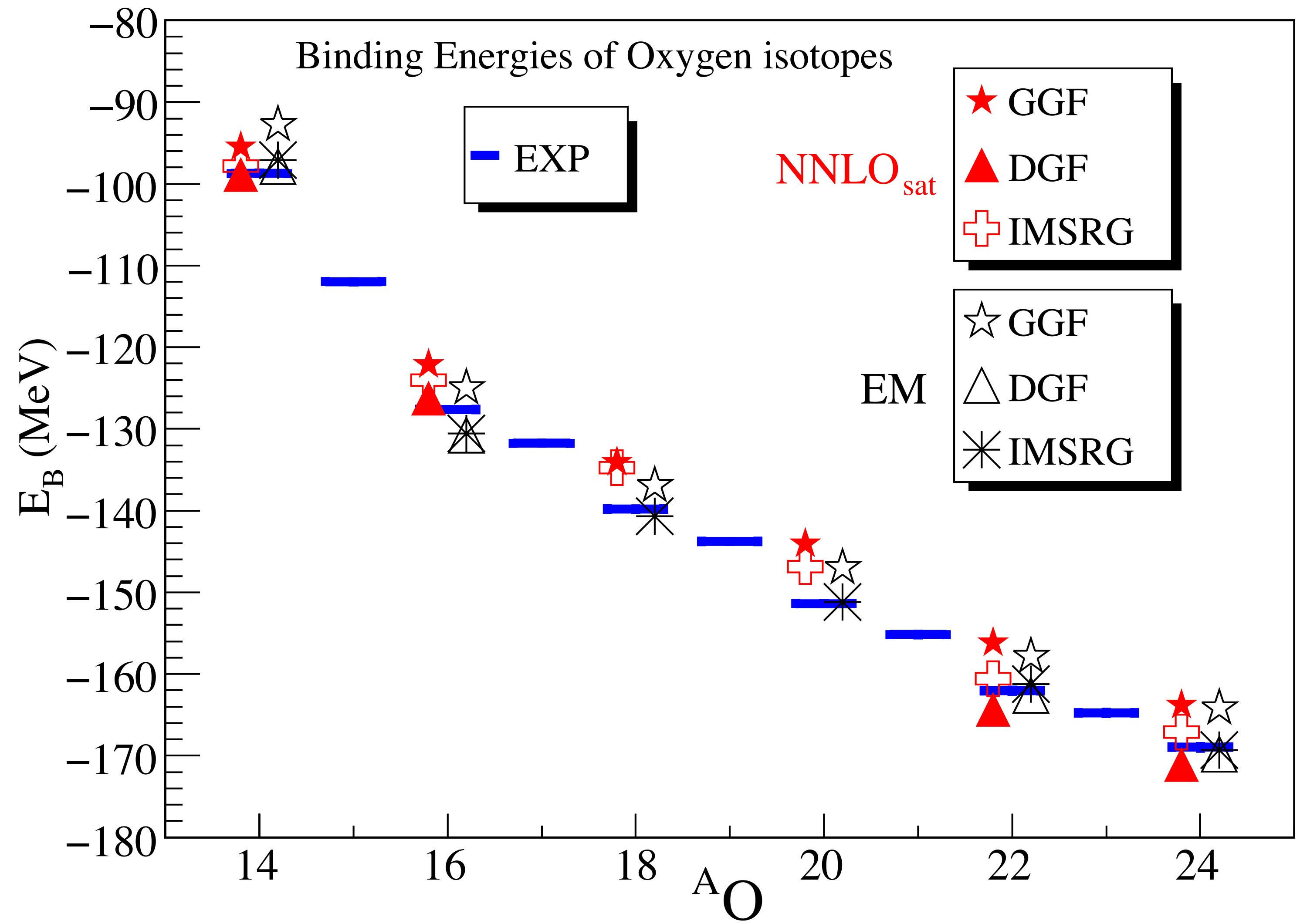
[Schirmer & Angonoa 1989]

Energy *independent* eigenvalue problem

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

- **Observables of *A*-body ground state** (both N & Z even)
- **Spectroscopic** information on $A\pm1$ systems

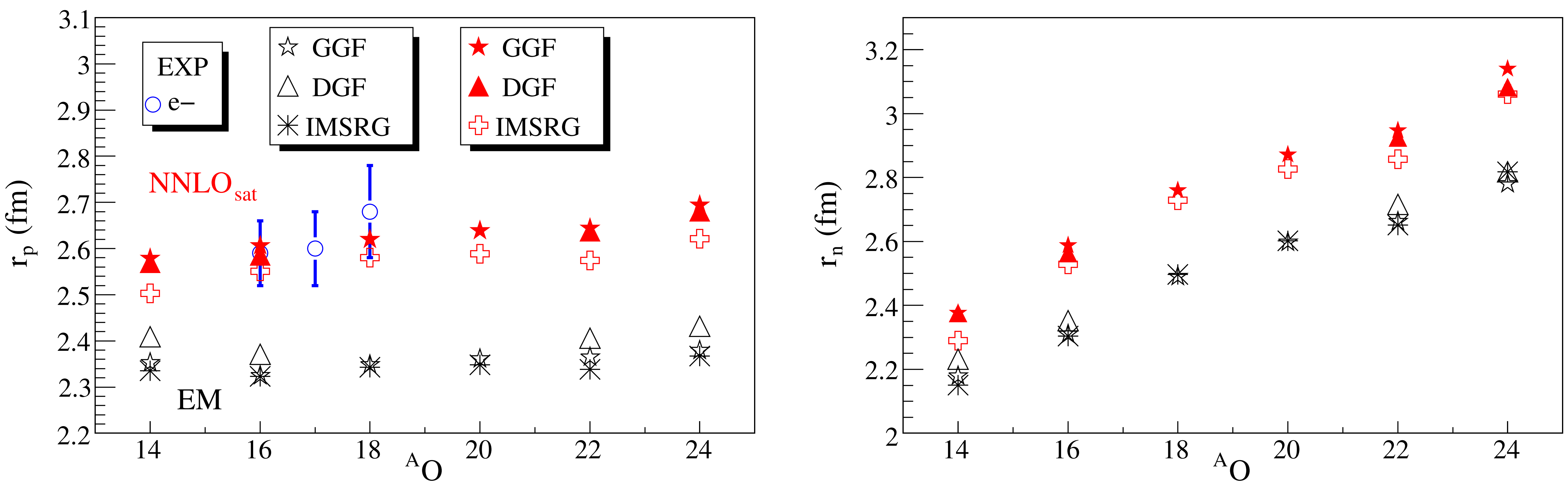
Oxygen energies and motivations



- **EM** and **NNLO$_{sat}$** perform similarly along O binding energies
  - Comparable spread between different many-body schemes for the two interactions
  - Fair agreement with experiment (including drip-line)

- **EM** known to lead to a poor reproduction of radii [see e.g. Cipollone *et al*. 2015, …]

Oxygen point-proton and point-neutron radii



- ⦿ **Uncertainty** from using different many-body schemes achieve is
  - ○ **smaller than experimental uncertainty**
  - ○ **smaller than the one associated the use of different interactions**

- ⦿ Point-proton radii (deduced from (e,e) scattering) available only for stable $^{16\text{-}18}$O

  ➟ **matter radii**?

Evaluating matter radii

- **Hadronic probe necessary**
  - Elastic proton scattering
  - Nucleus-nucleus collisions

Modelling of the reaction mechanism needs to be under control

- Here matter radii are extracted from **angular distributions of (p,p) cross sections**
  - (p,p) cross sections computed in the Distorted Wave Born Approximation (DWBA)
  - Optical potential JLM $U_{JLM}(\rho, E) = \lambda_V V(\rho, E) + i\lambda_W W(\rho, E)$

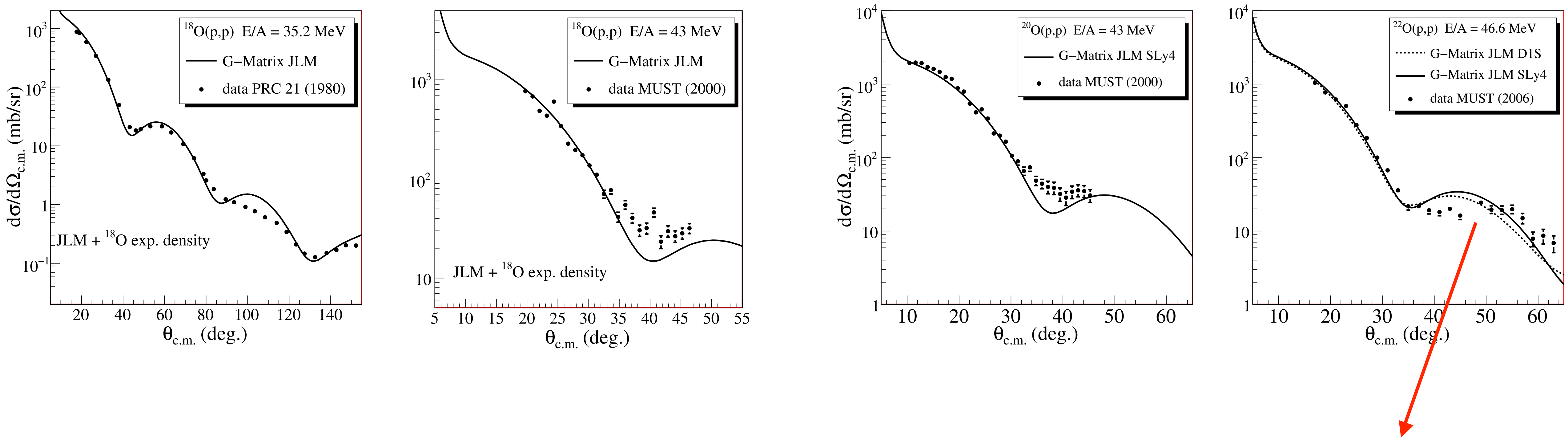
[Jeukenne, Lejeune & Mahaux 1977]

INPUTS
- Incident energy
- Proton and neutron densities

Evaluating matter radii

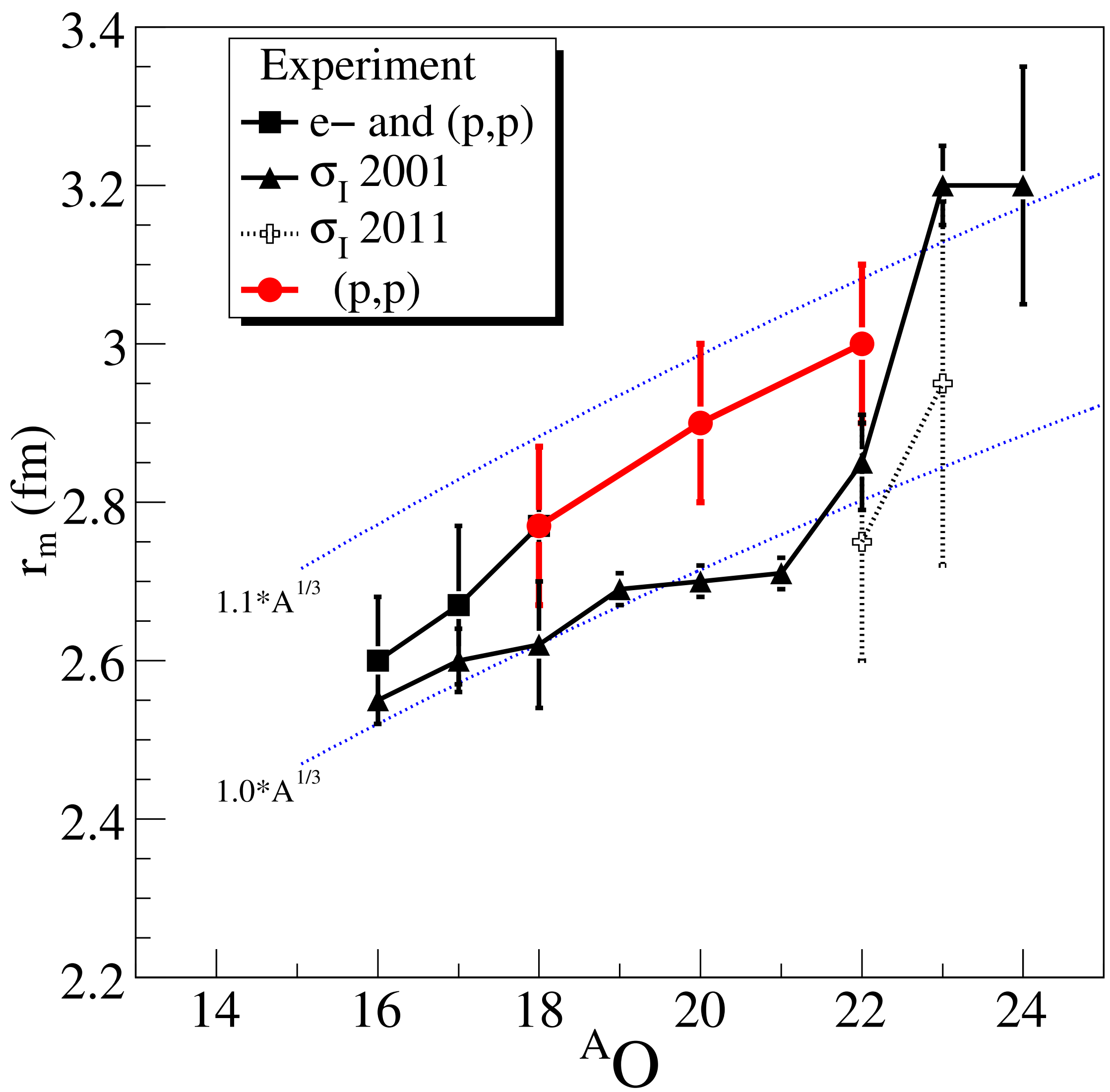
- **Matter radii** evaluated as follows

  1. "Experimental" densities are extracted from (e,e) for $^{16\text{-}18}O$
  2. DWBA with "experimental" densities validate the use of JLM potential for (p,p) data
  3. Skyrme densities are benchmarked on (p,p) in $^{16\text{-}18}O$
  4. DWBA calculations with Skyrme densities are extended to neutron-rich isotopes



➟ **uncertainty of 0.1 fm** from the use of different microscopic densities (consistent with older analyses on stable nuclei)

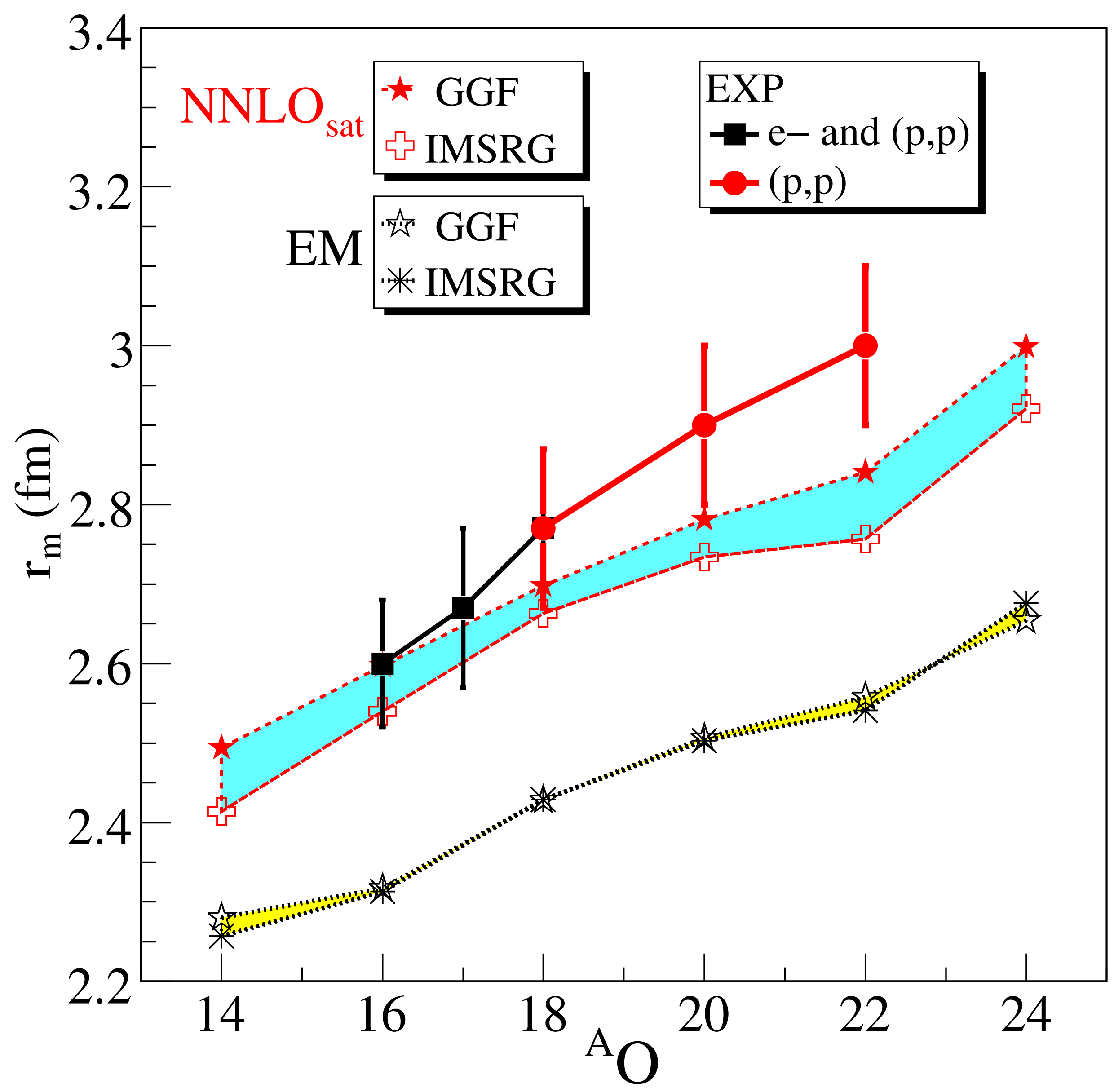
Oxygen matter radii: exp. vs exp.



A	16	17	18	20	22
r_p	2.59 (7)	2.60 (8)	2.68 (10)		
r_m (σ_I)	2.54 (2)	2.59 (5)	2.61 (8)	2.69(3)	2.88(6)
r_m (p,p)	2.60 (8)	2.67 (10)	2.77 (10)	2.9 (1)	3.0 (1)

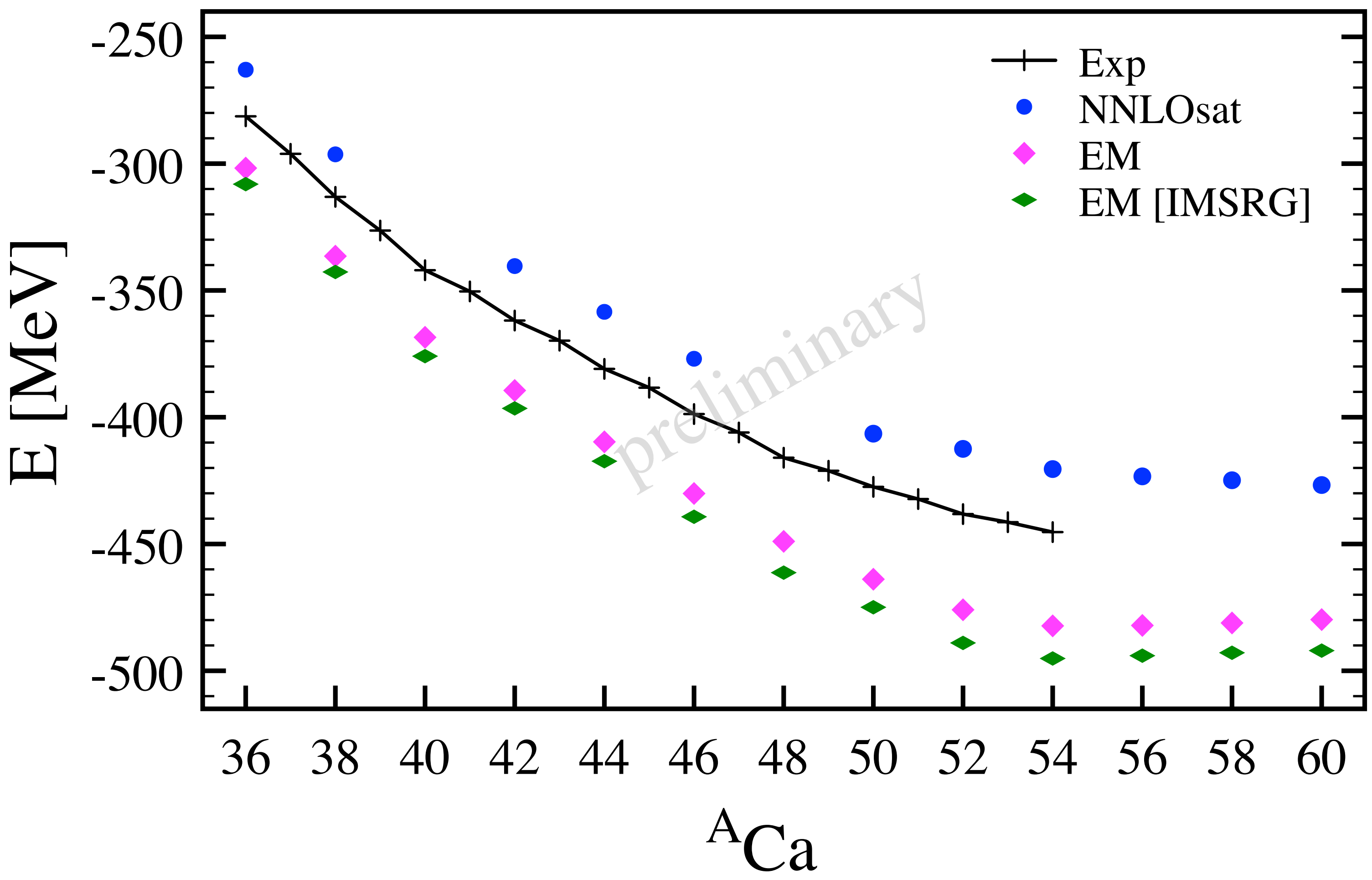
- (p,p) analysis in agreement with (e,e) benchmarks in $^{16\text{-}18}$O
- Alternative evaluation from **interaction cross section** (σ_I)
  - 2001 analysis likely to underestimate systematic errors [Ozawa *et al*. 2001]
  - 2011 new experiment with $^{22\text{-}23}$O [Kanungo *et al*. 2011]

Oxygen matter radii: exp. vs theory



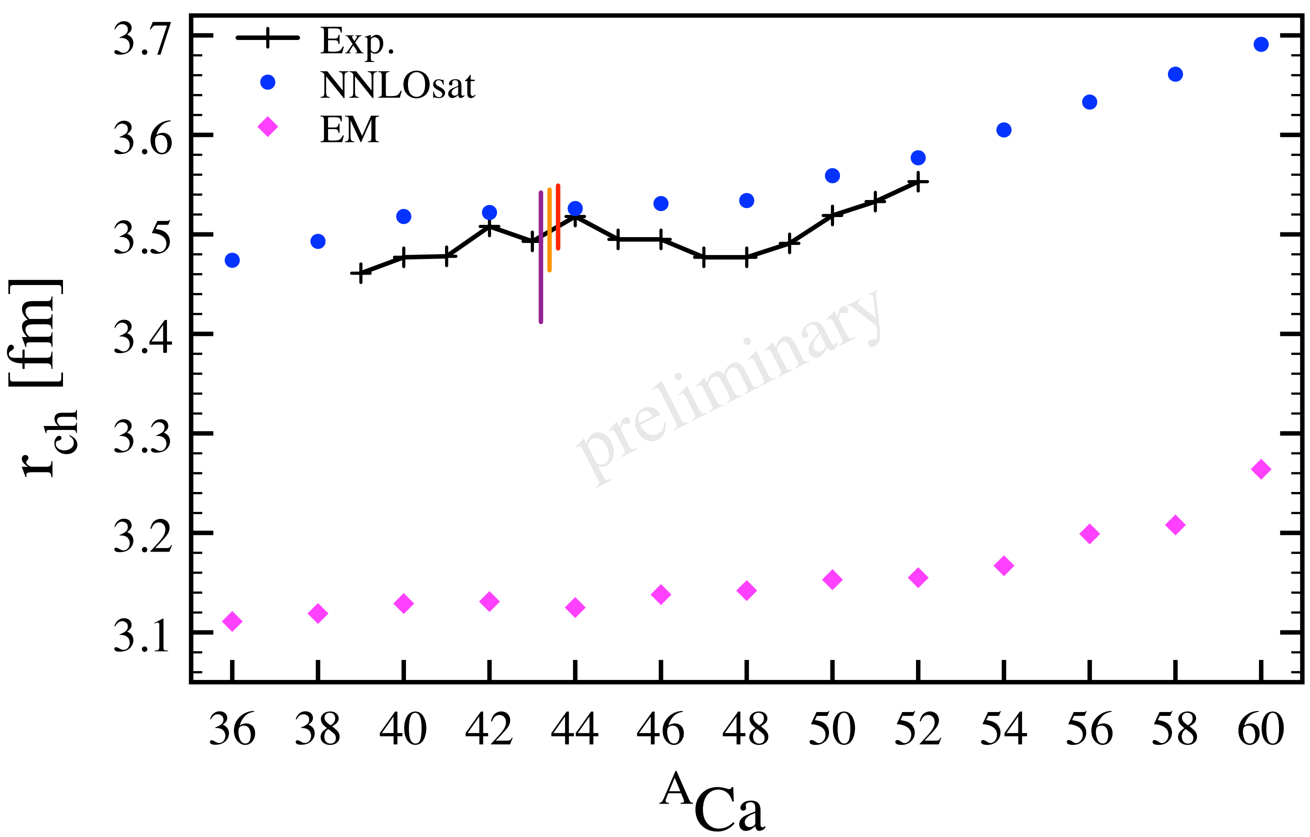
- Clear **improvement in absolute** (^{16}O r_{ch} in NNLO$_{sat}$ fit)
- Somewhat **similar *N* dependence**

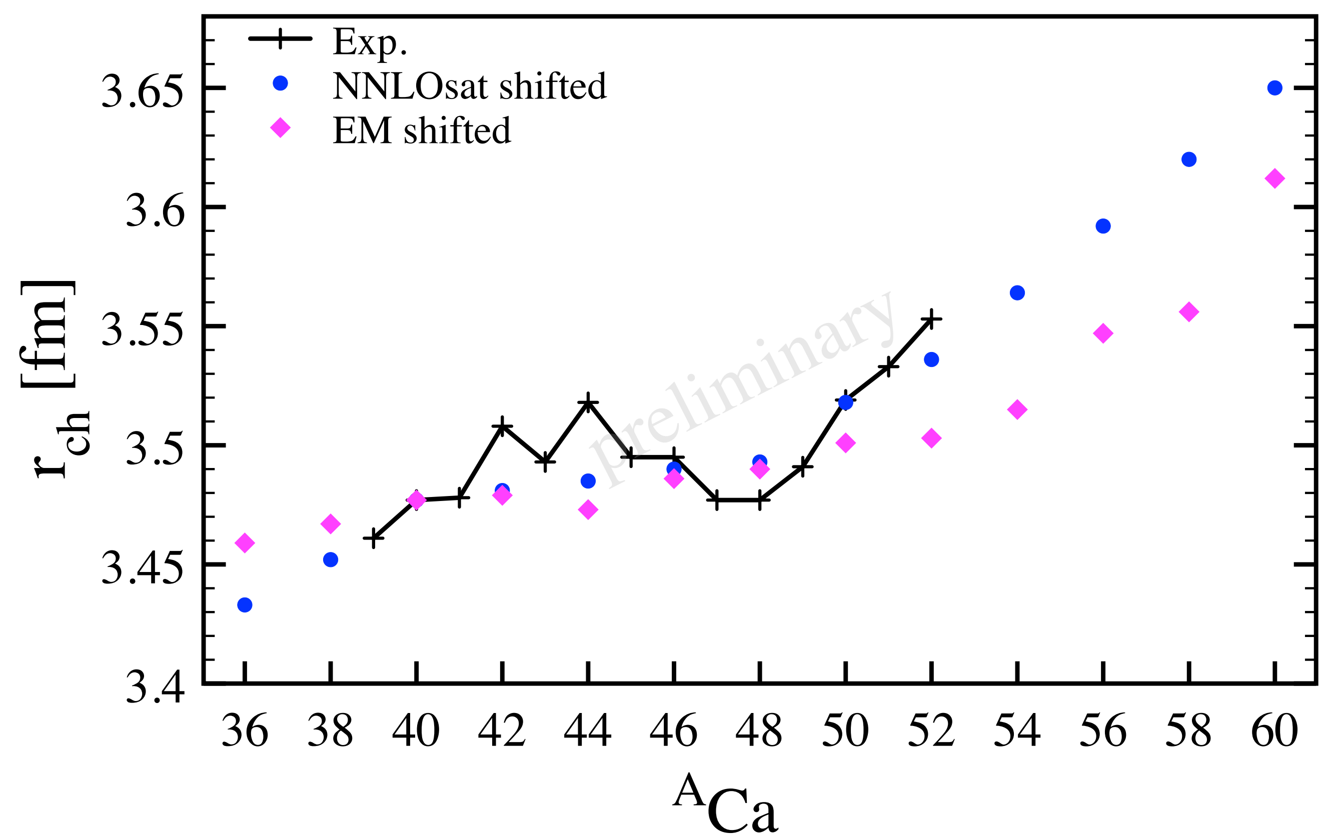
Calcium binding energies



- **NNLO$_{sat}$ corrects overbinding**
- Two-neutron separation energies:
    - comparable to EM for light isotopes
    - drip-line pushed to higher masses
- **Many-body uncertainties** to be further assessed

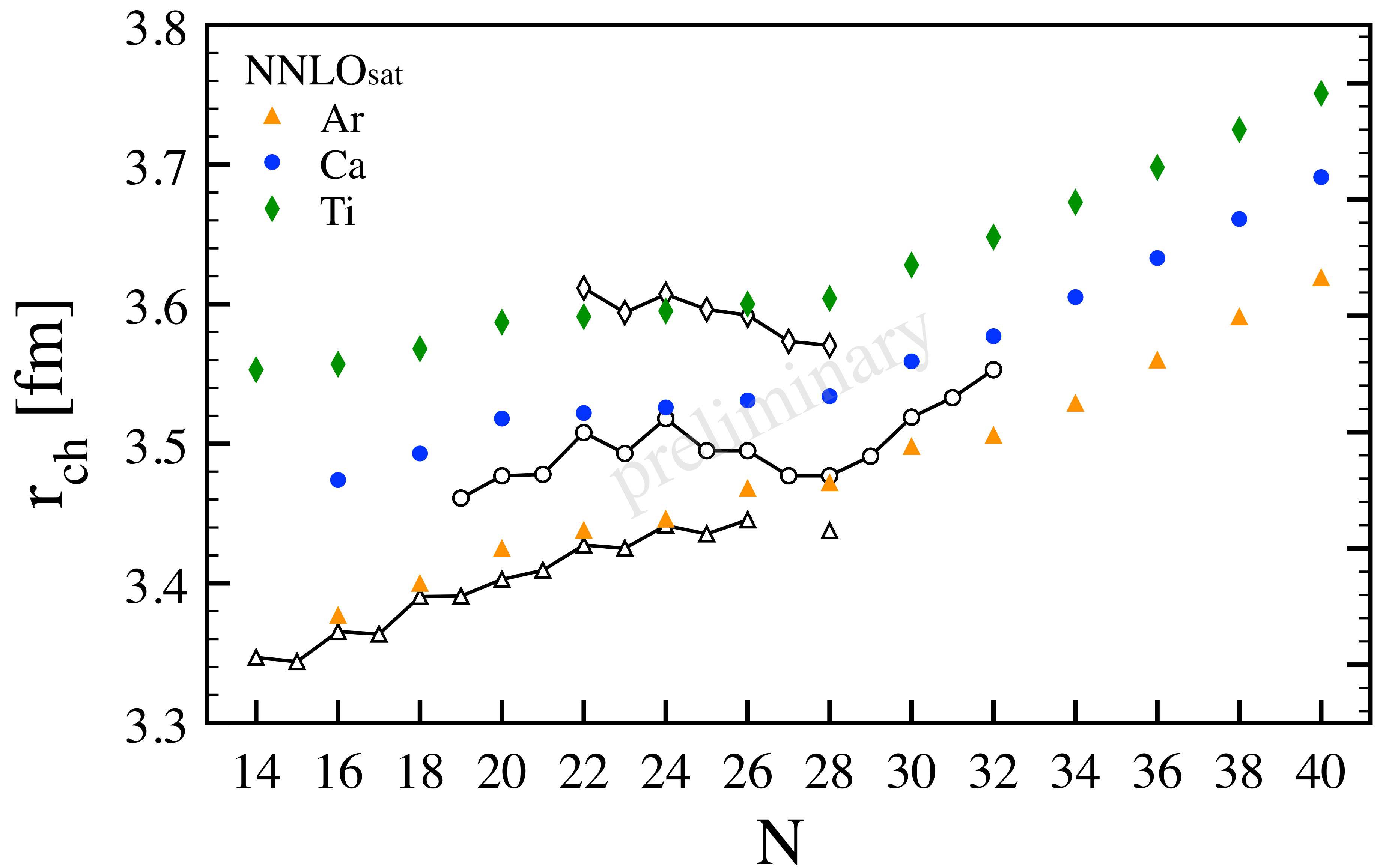
Calcium charge radii





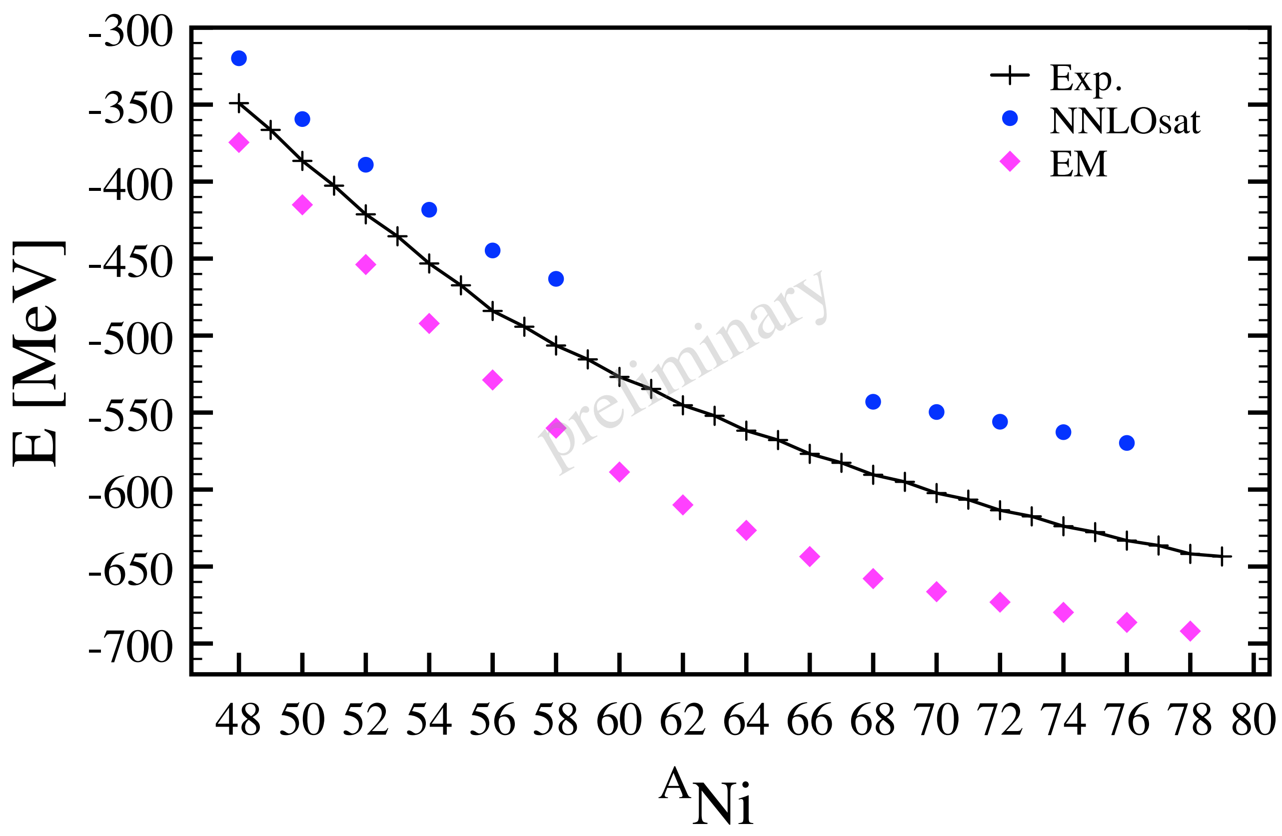
- NNLO$_{sat}$: charge radii improve both in **absolute** and **relative**
- Cf. new measurements of ^{49,51,52}Ca and similar CC calculations [Garcia Ruiz *et al.* 2016]
- Parabolic behaviour between ^{40}Ca and ^{48}Ca remains a challenge
- Odd-even staggering? (*work in progress*)

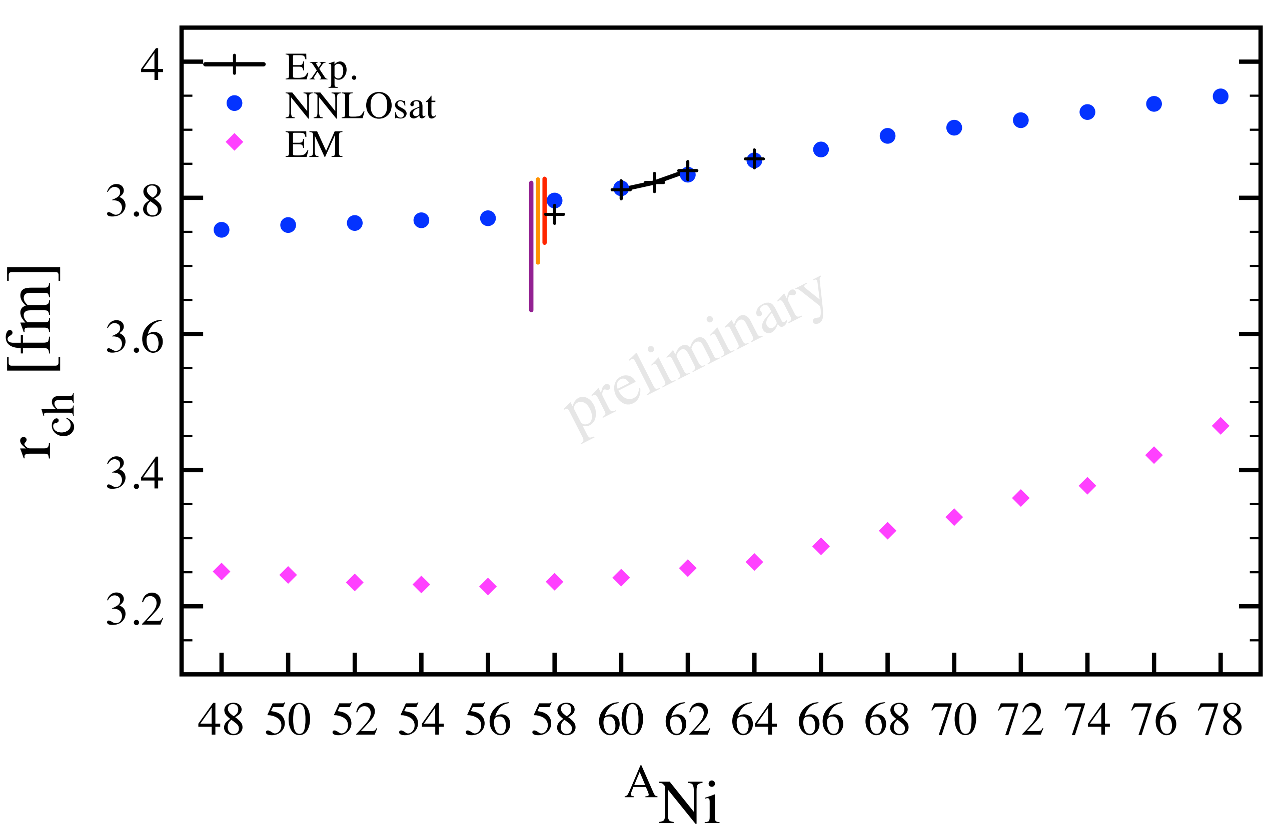
Charge radii around Z=20



- Hints of the nontrivial behaviour as a function of *N* and *Z*
- More delicate to disentangle effects of missing many-body correlations/interactions

Up to nickel





- Improvement seen around *Z*=20 is **confirmed in nickel**
- Many-body convergence to be assessed with ADC(3) calculations

Summary

- **Matter radii** complement energy systematics along the oxygen chain
  - **(p,p) scattering** data provides precious information for unstable isotopes
  - (p,p) evaluation of matter radii mostly inconsistent with σ_I
  - Different many-body schemes provide consistent results
  - $NNLO_{sat}$ falls short in reproducing (p,p) matter radii towards the drip-line

- Unconventional **$NNLO_{sat}$** significantly improves on EM deficiencies
  - **Overbinding** corrected
  - Nuclei have the **right size**, isospin dependence still to be refined?
  - Other observables?
  - How to proceed **systematically**?

Appendix

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

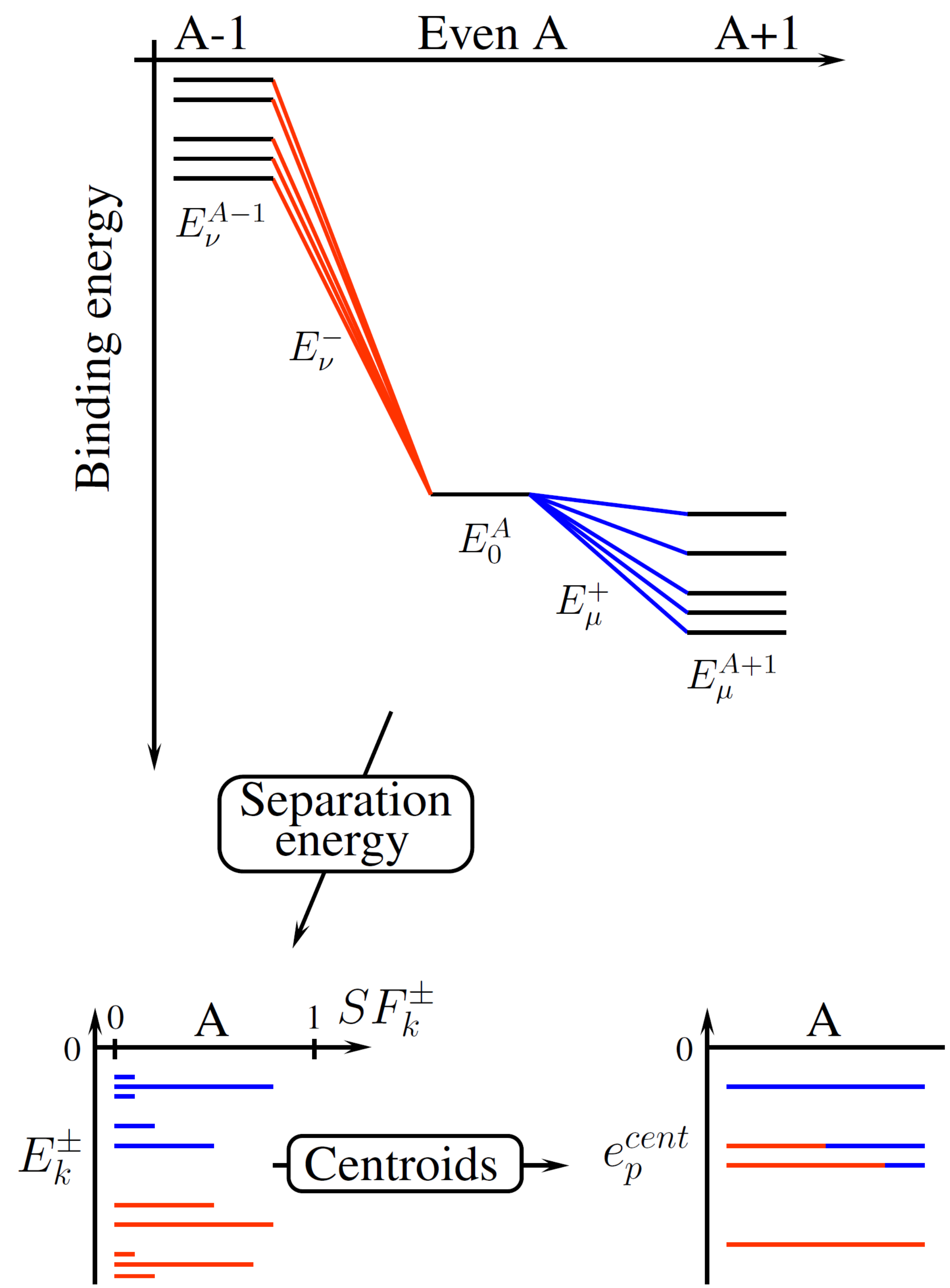
where
$$\begin{cases} \mathcal{U}^{k*}_a \equiv \langle \Psi_k | a^\dagger_a | \Psi_0 \rangle \\ \mathcal{V}^{k*}_a \equiv \langle \Psi_k | \bar{a}_a | \Psi_0 \rangle \end{cases}$$

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

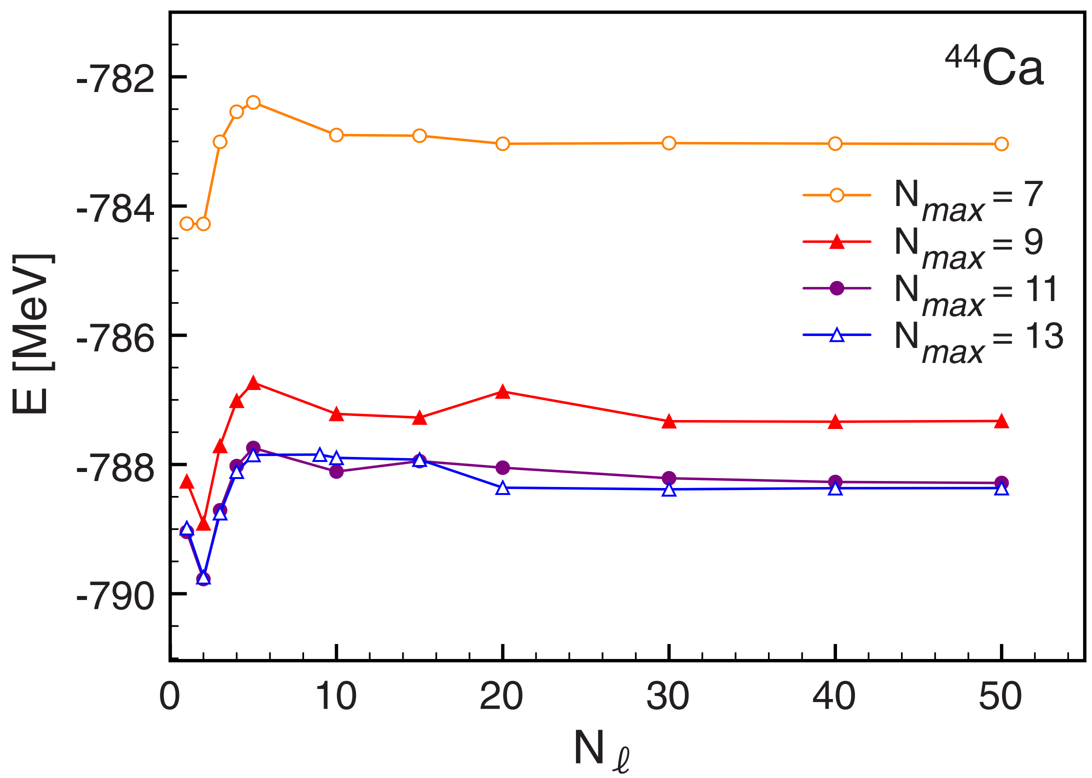
$$SF^+_k \equiv \sum_{a \in \mathcal{H}_1} \left| \langle \psi_k | a^\dagger_a | \psi_0 \rangle \right|^2 = \sum_{a \in \mathcal{H}_1} \left| \mathcal{U}^k_a \right|^2$$

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

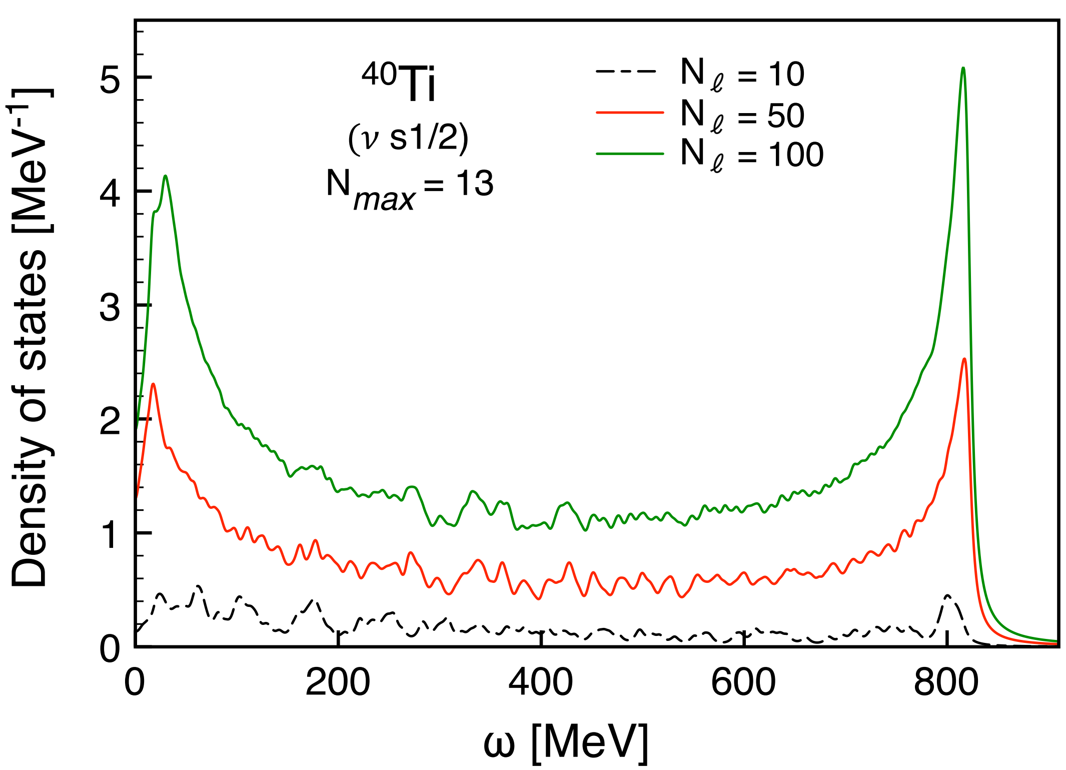


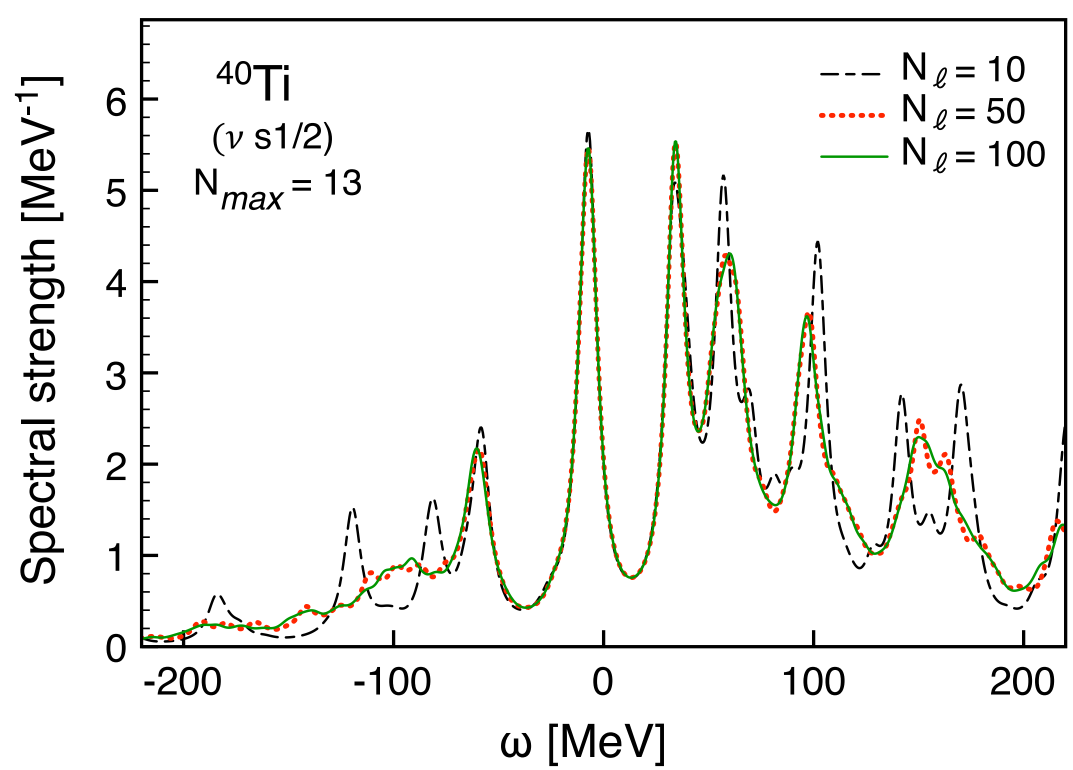
[figure from J. Sadoudi]

Krylov projection



- Multi-pivot algorithm (# states ~ 10 N_ℓ)
- Well converged for N_ℓ ~ 50
- Independent of N_{max}
- Spectral strength quickly converges around the Fermi surface



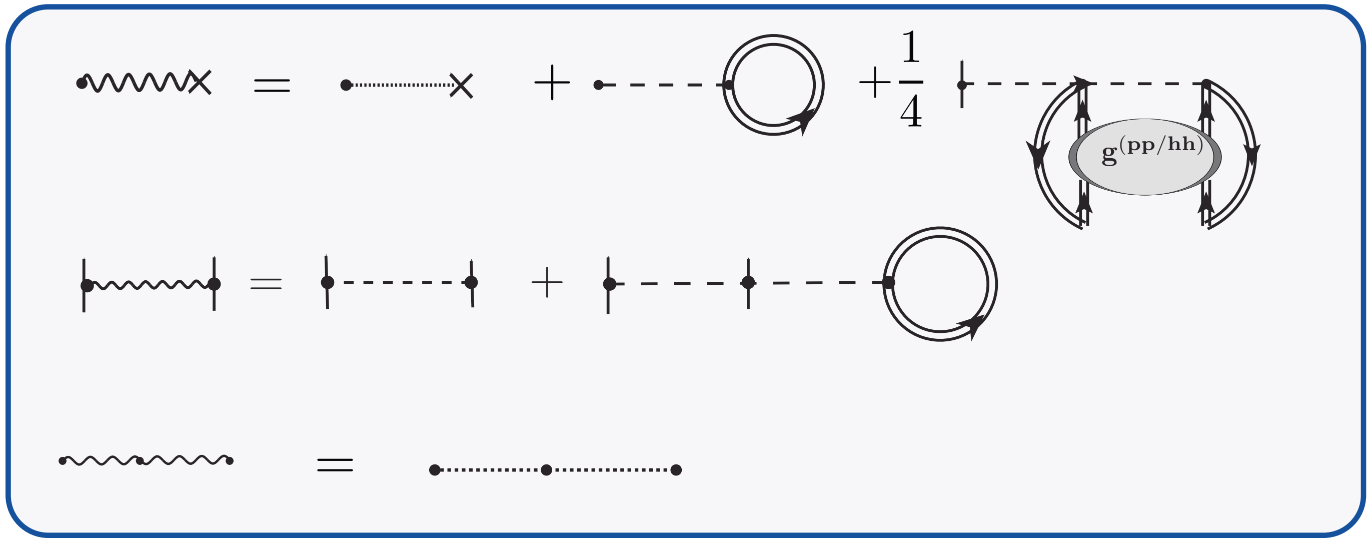


[Somà, Barbieri & Duguet 2014]

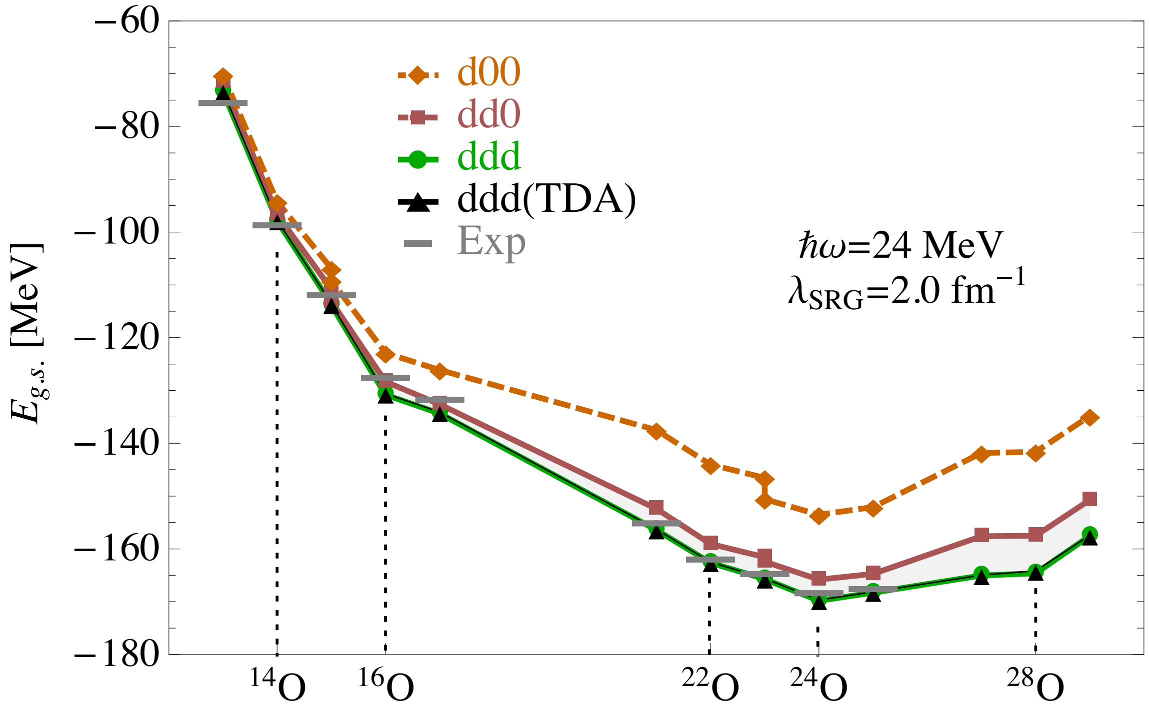
Three-body forces

- 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



[Carbone, Cipollone *et al.* 2013]



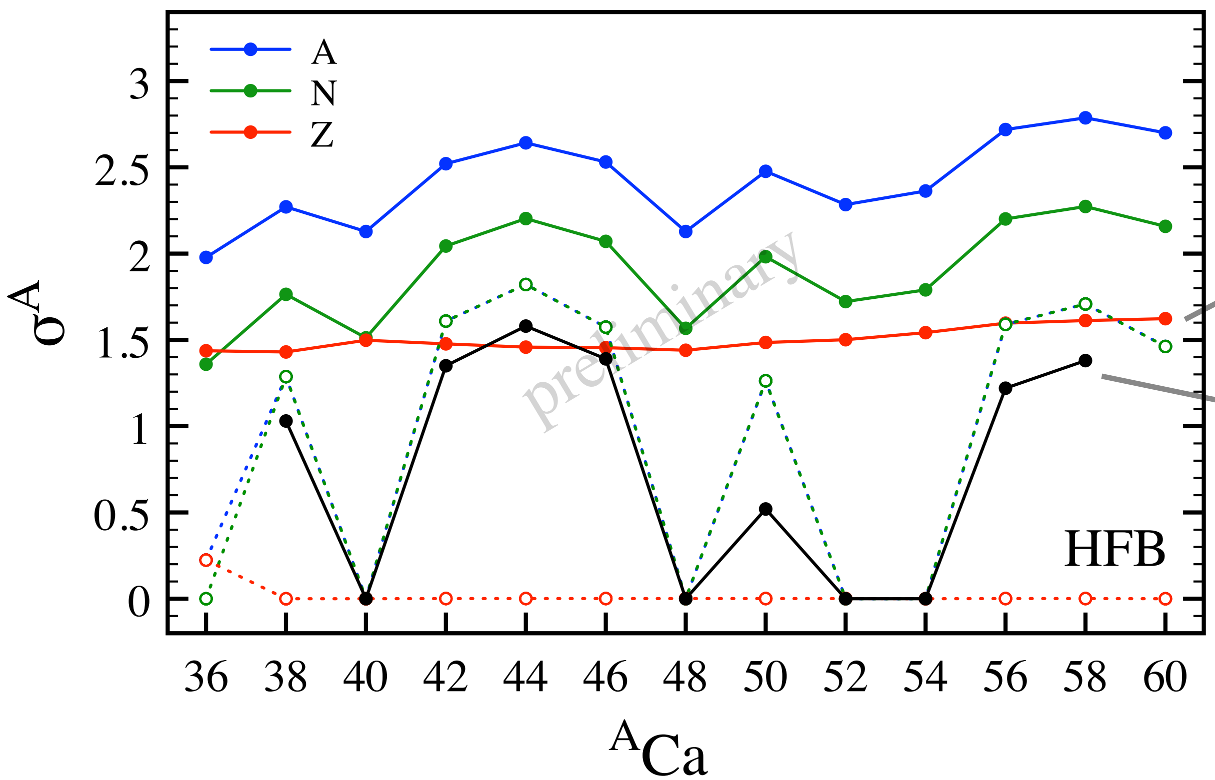
➟ Use of dressed propagators provides extra correlations

Particle-number variance

- Gorkov GF calculations break particle number symmetry → $\sigma_A = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$
- Breaking has two sources:

  1) Reference state mixes different A

  2) Green's function formalism itself explores Fock space



GF breaking evident in protons

After subtracting GF part

Odd-even systems

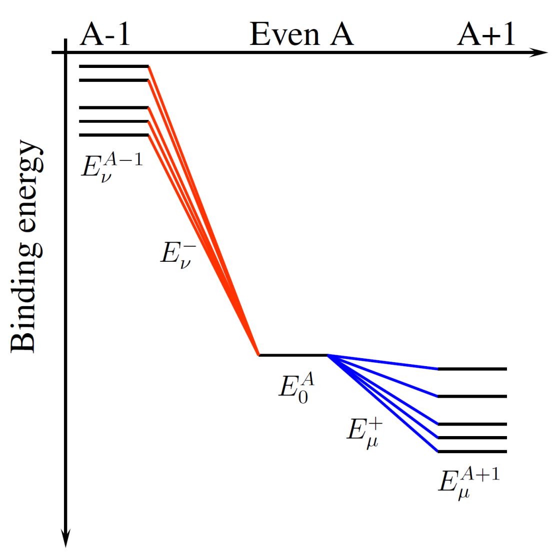
⊙ Current implementation targets $J^{\pi} = 0^{+}$ states

➟ Equations simplify: j-coupled scheme, block-diagonal structure, ...

⊙ Different possibilities to compute odd-even g.s. energies:

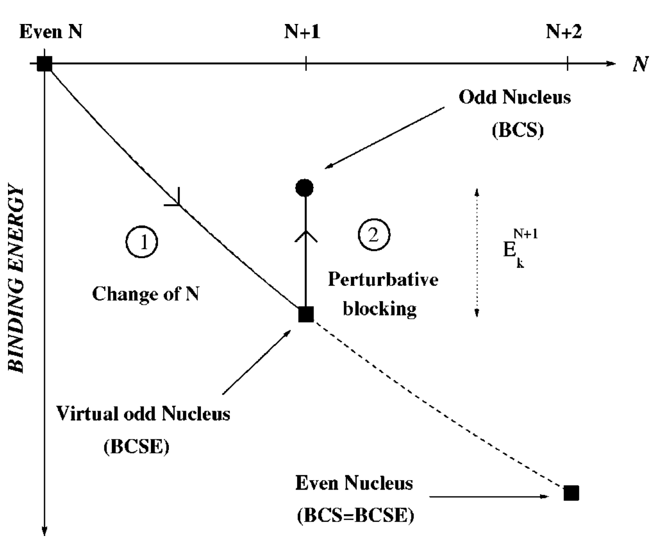
① From separation energies

➟ Either from A-1 or A+1



② From fully-paired even number-parity state

➟ "Fake" odd-A plus correction



[Duguet *et al.* 2001]

Two methods agree within 2-300 keV