Green's function approach to the nuclear many-body problem

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RPA workshop
Paris, 2 May 2017

Collaborators

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- Carlo Barbieri (University of Surrey, UK)
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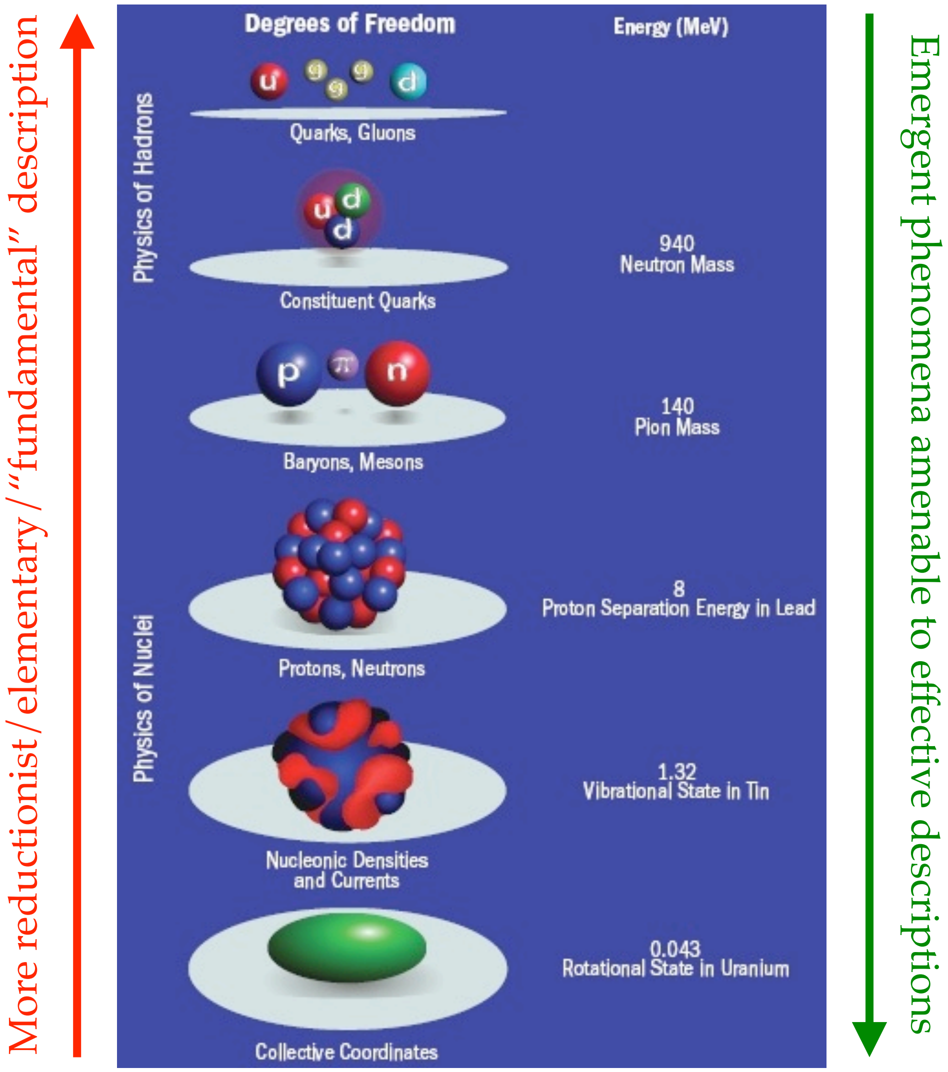
Outline

- Ab initio nuclear many-problem: state of the art
- Self-consistent Green's functions: current implementations and issues
- Benchmarks & modelling of nuclear Hamiltonians
- Study of potential bubble nucleus Si34

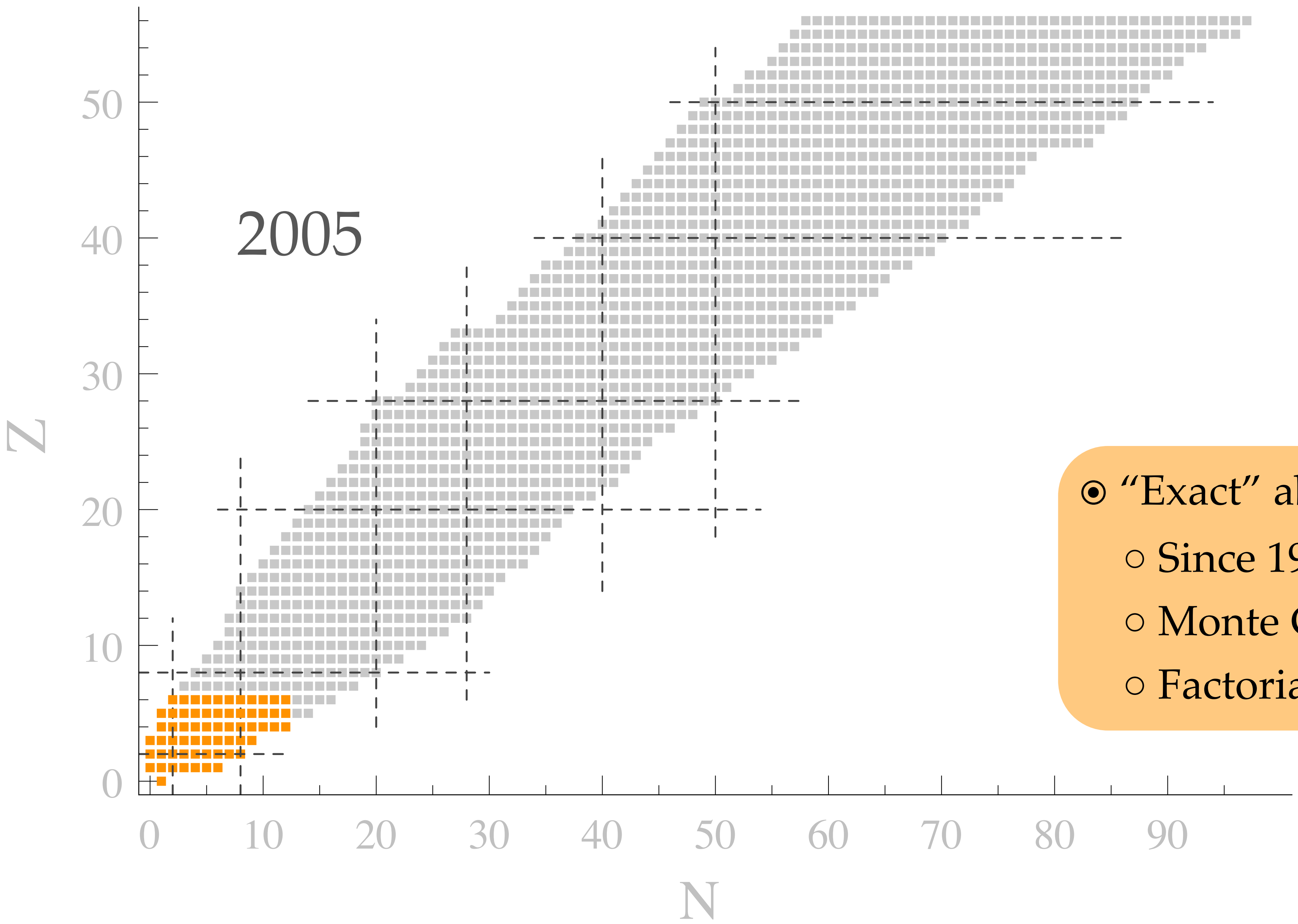
Ab initio nuclear *A*-body problem



- **Nucleus:** system of *A* structure-less nucleons
- Nucleons interact via **inter-nucleon** (2N, 3N, ..) **forces**
- Hamiltonian *H* from an **effective field theory** (EFT)
  - Systematic construction of *H* for a given set of d.o.f.
  - Symmetries of underlying theory (here QCD) built in
  - Couplings fixed by underlying theory or exp. data
  - EFTs for nuclear systems: **pionless** or **chiral EFT**
- Solve $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$ (as well as you can)

- **Difficulties**: costly many-body methods, highly nontrivial construction of interactions
- **Benefits**: systematic improvement, assessment of errors ➟ controlled extrapolations
- **Questions**: does it work, to what accuracy and which are the limits of applicability?

Evolution of ab initio nuclear chart



- ⊙ "Exact" ab initio approaches
  - ○ Since 1980's
  - ○ Monte Carlo, CI, …
  - ○ Factorial scaling

Evolution of ab initio nuclear chart

- ⦿ Ab initio approaches for closed-shell nuclei
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  - ○ SCGF, CC, IMSRG
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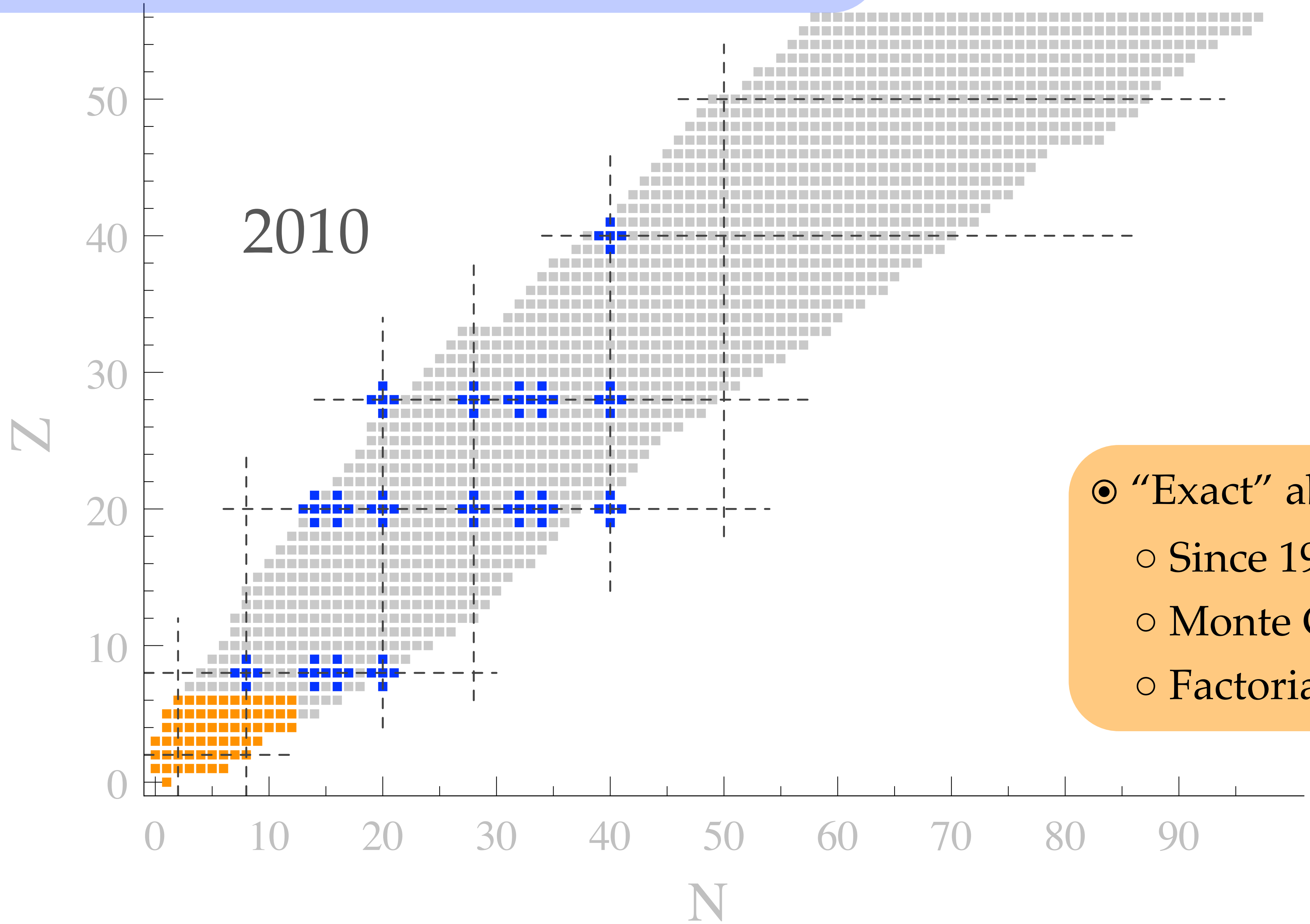

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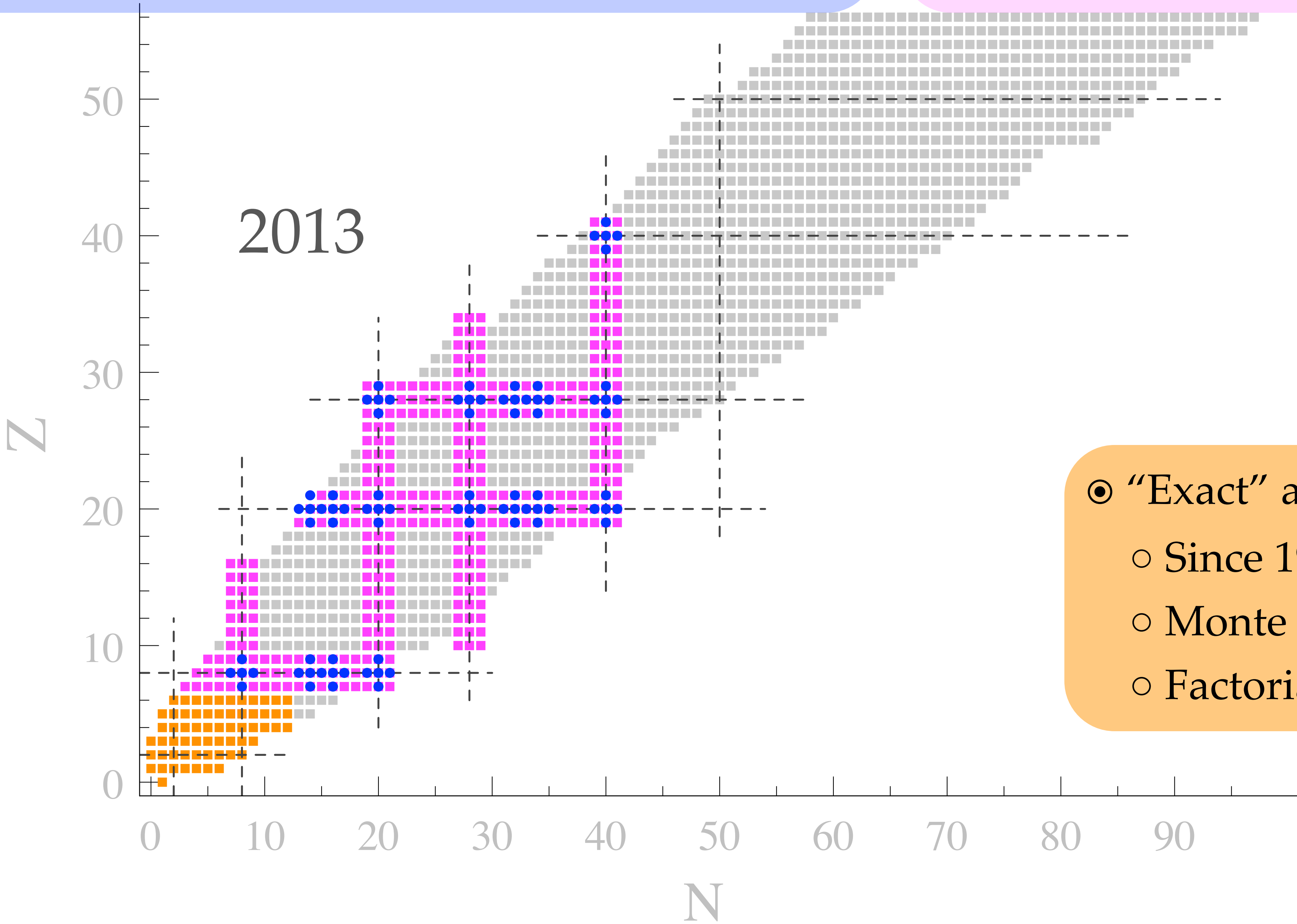

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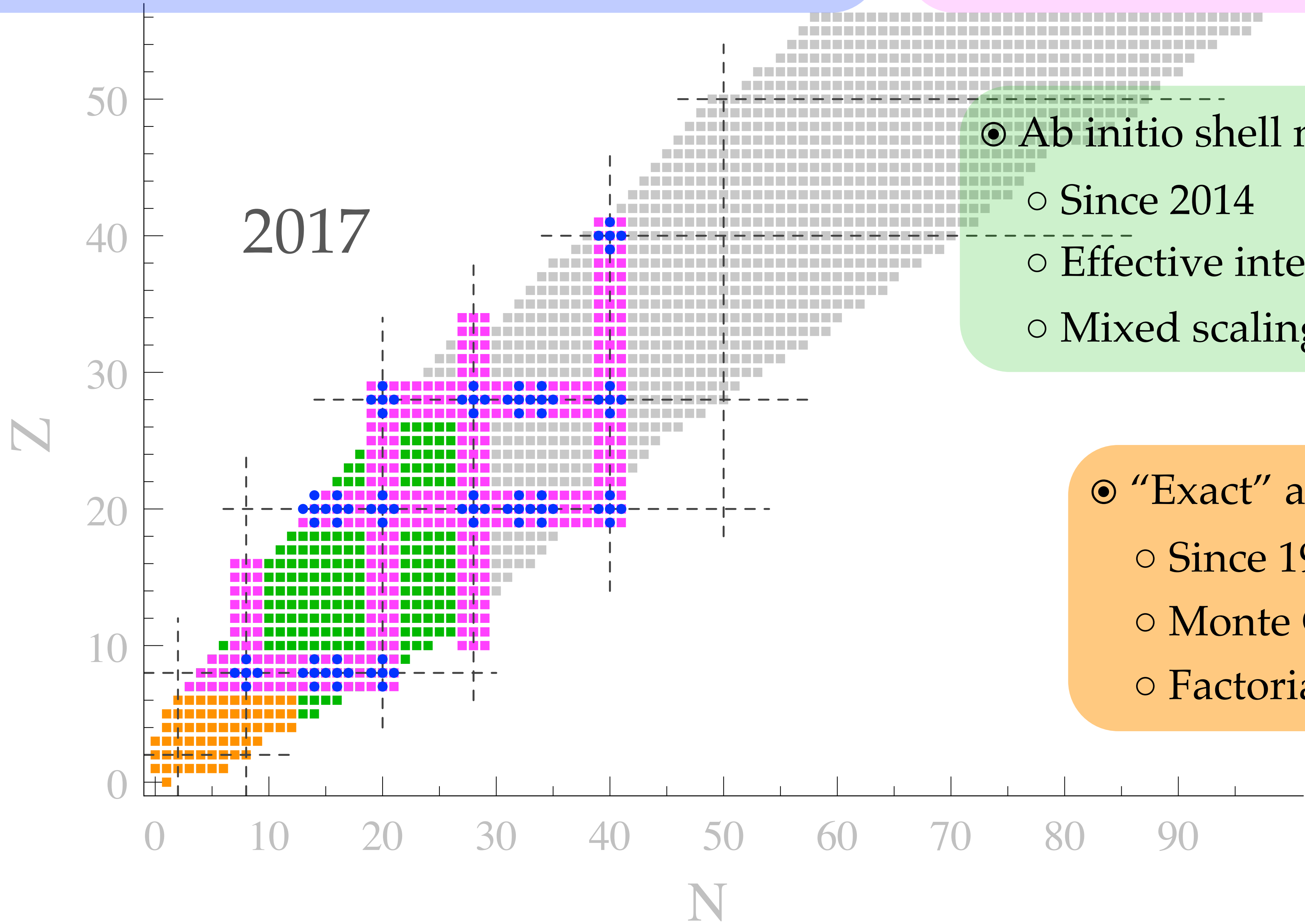

- ⊙ Ab initio shell model
  - ○ Since 2014
  - ○ Effective interaction via CC/IMSRG
  - ○ Mixed scaling

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Self-consistent Green's function approach

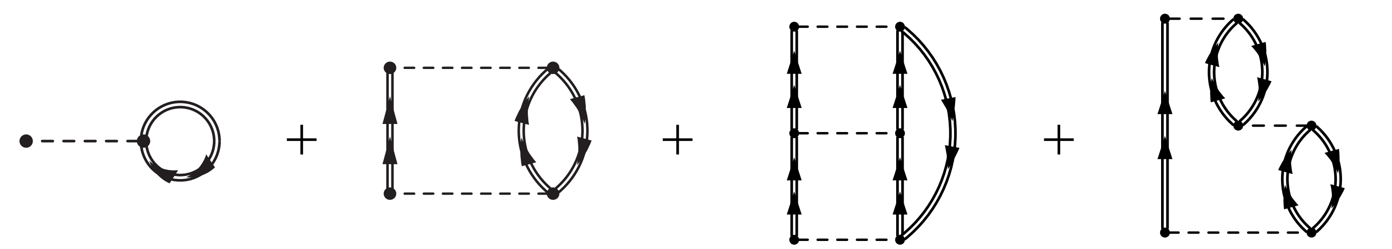
- **Solution of the *A*-body Schrödinger equation** $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$ **achieved by**

  1) Rewriting it in terms of **1-, 2-, …. *A*-body objects** G_1=G, G_{2}, … G_A (**Green's functions**)

  2) Expanding these objects in perturbation (in practise **G** ➟ **one-body observables**, etc..)

  - **Self-consistent** schemes resum (infinite) subsets of perturbation-theory contributions

Self-energy expansion $\boldsymbol{\Sigma}$ =



$+ \ldots$

Dyson equation $\mathbf{G} = \mathbf{G^0} + \mathbf{G^0}\,\boldsymbol{\Sigma}\,\mathbf{G}$

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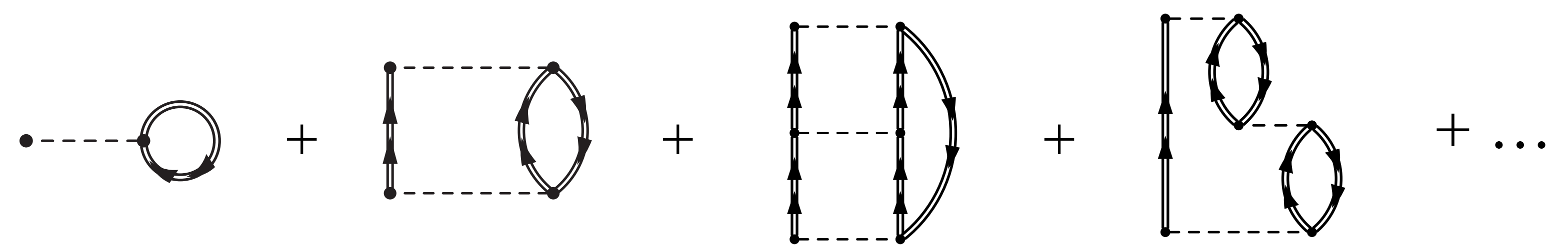
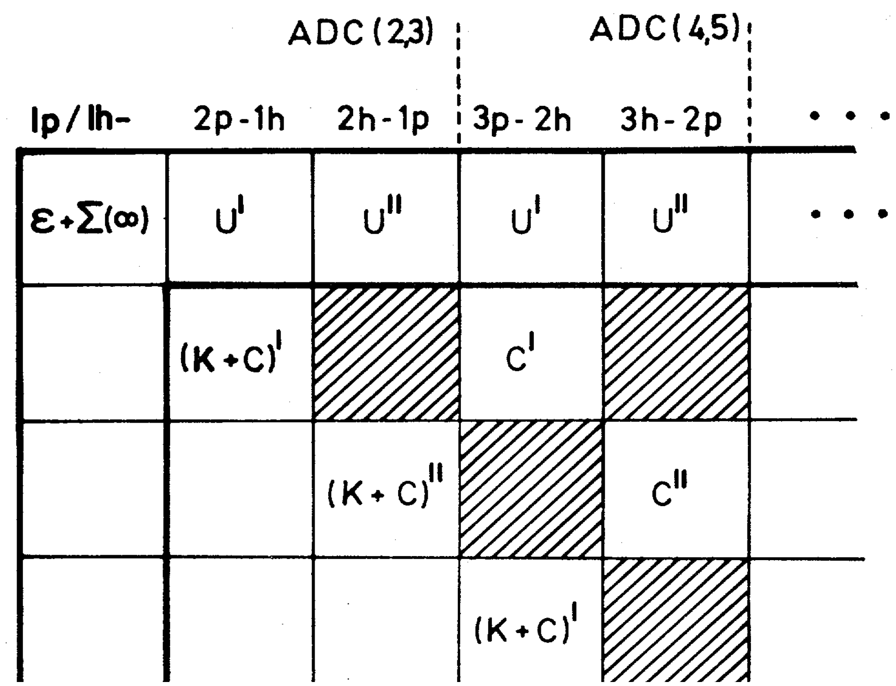


Dyson equation $\mathbf{G} = \mathbf{G^0} + \mathbf{G^0}\,\boldsymbol{\Sigma}\,\mathbf{G}$

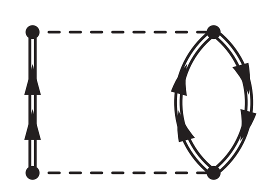
- **G** → ground-state properties of even-even A + spectra of odd-even neighbours
  - ○ Advanced resummation schemes exist
  - ○ Some operators routinely computed, more to be implemented
  - ○ Optical potential for nucleon-nucleus scattering obtainable directly from Σ
- **G_2 (polarisation propagator)** → excited spectrum of even-even A
  - ○ To be developed

Self-energy approximation schemes

- **Algebraic Diagrammatic Construction (ADC)** [Schirmer, Cederbaum & Walter 1983]
  - Exploits spectral form of self-energy to reformulate its expansion into an algebraic form
  - ADC(n) includes complete n-th order (dressed) perturbation theory diagrams for G
  - Results in Hermitian eigenvalue problems within limited spaces of N±1 systems



ADC(2)



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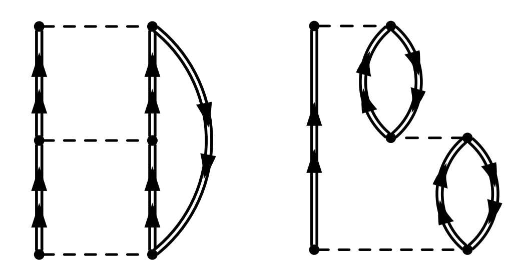

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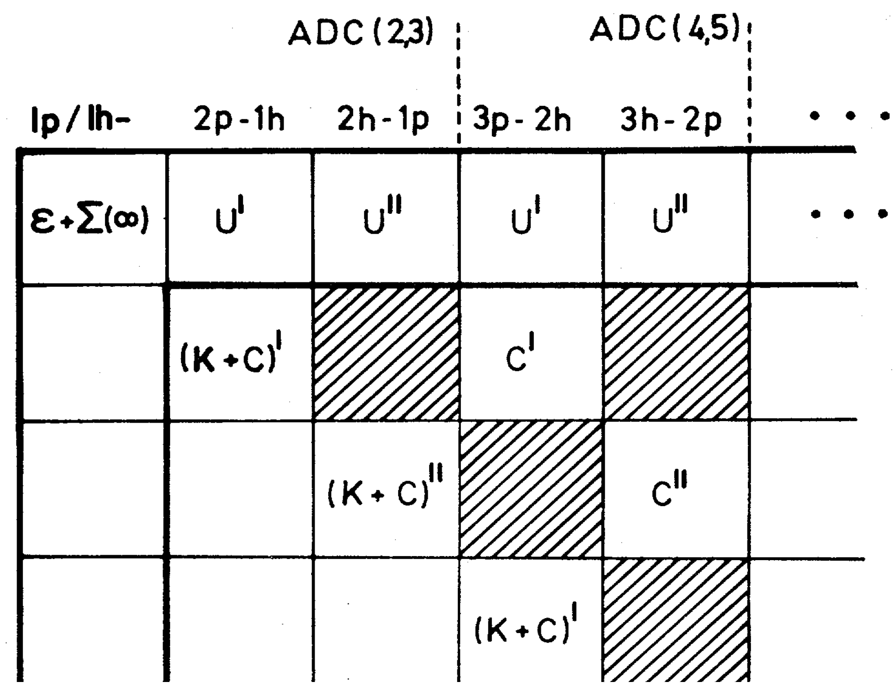

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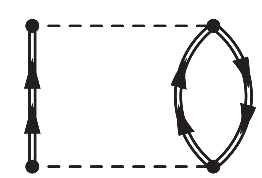
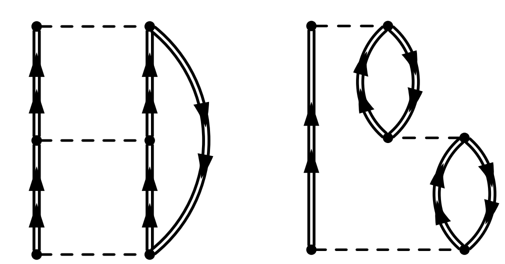
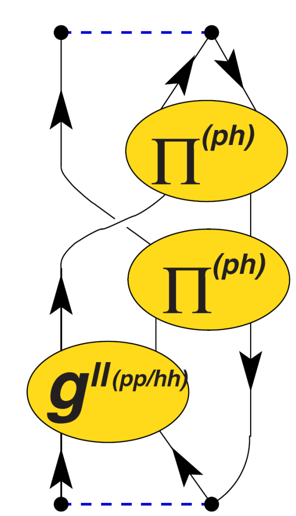


ADC(3)



…

- **Faddeev-RPA** [Barbieri & Dickhoff 2007]
  - Each ph and pp/hh channel is computed separately
  - Two-body propagators are subsequently coupled to a third line
  - All-order summation through a set of Faddeev equations



Ab initio methods for open-shell nuclei

- Standard expansion schemes fail when dealing with, e.g., pairing instabilities
  ➟ Idea: use **symmetry breaking** (particle number) to account for pairing

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

$$|\Psi_0^A\rangle = \Omega_0|\phi\rangle$$

where both Ω_0 and $|\phi\rangle$ break symmetries

$$E_0^A = \frac{\langle\phi|H\Omega_0|\phi\rangle}{\langle\phi|\Omega_0|\phi\rangle}$$

- **Gorkov self-consistent Green functions (GGF)**
  [Somà, Duguet, Barbieri 2011]
- Multi-reference IMSRG
  [Hergert *et al.* 2013]
- **Bogoliubov coupled-cluster (BCC)**
  [Signoracci *et al.* 2015]
- **Symmetry-restored BCC**
  [Duguet 2015; Duguet, Signoracci 2016]

- Revisit basic/investigate new questions from an ab initio perspective
  - **Emergence of magic numbers** and their evolution
  - **Limits of stability** on neutron-rich side beyond Z=8
  - **Mechanism for nuclear superfluidity**
  - Emergence and evolution of quadrupole collectivity
  - Role and validation of AN forces

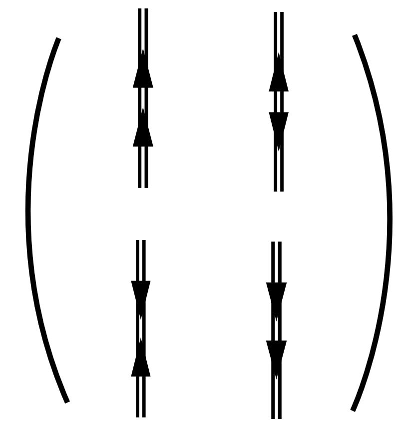
Gorkov-Green's functions

- Start expansion from symmetry-breaking reference $|\Psi_0\rangle \equiv \sum_{A}^{\text{even}} c_A \, |\psi_0^A\rangle$ [Gorkov 1958]

Dyson/Gorkov equation

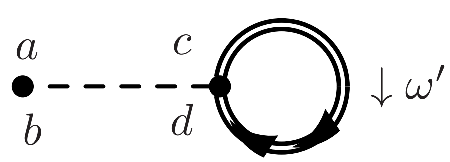
$$\mathbf{G}_{ab}(\omega) = \mathbf{G}^{(0)}_{ab}(\omega) + \sum_{cd} \mathbf{G}^{(0)}_{ac}(\omega)\, \mathbf{\Sigma}^{\star}_{cd}(\omega)\, \mathbf{G}_{db}(\omega)$$

$$\mathbf{G}_{ab} = \begin{pmatrix} G^{11}_{ab} & G^{12}_{ab} \\ G^{21}_{ab} & G^{22}_{ab} \end{pmatrix} =$$

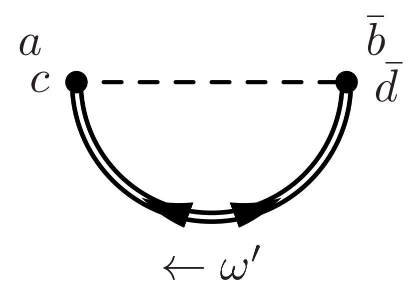


- Current self-energy truncation: **first**- and **second-order** diagrams [Somà, Duguet & Barbieri 2011]

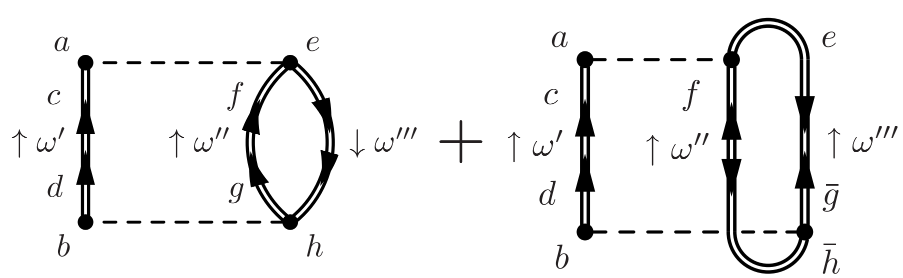
$\Sigma^{11\,(1)}_{ab} =$



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



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



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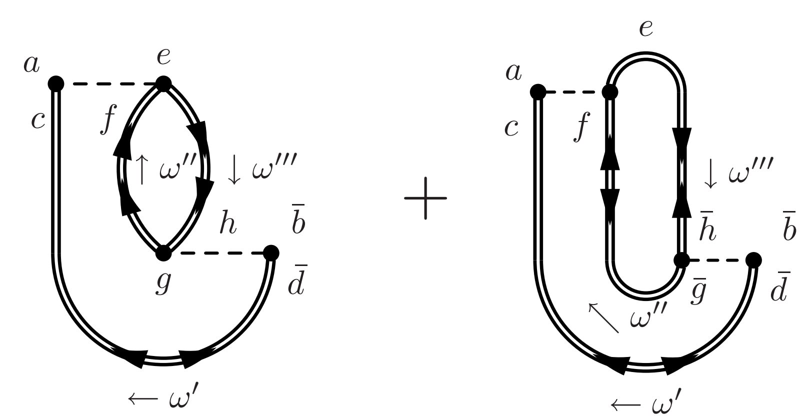
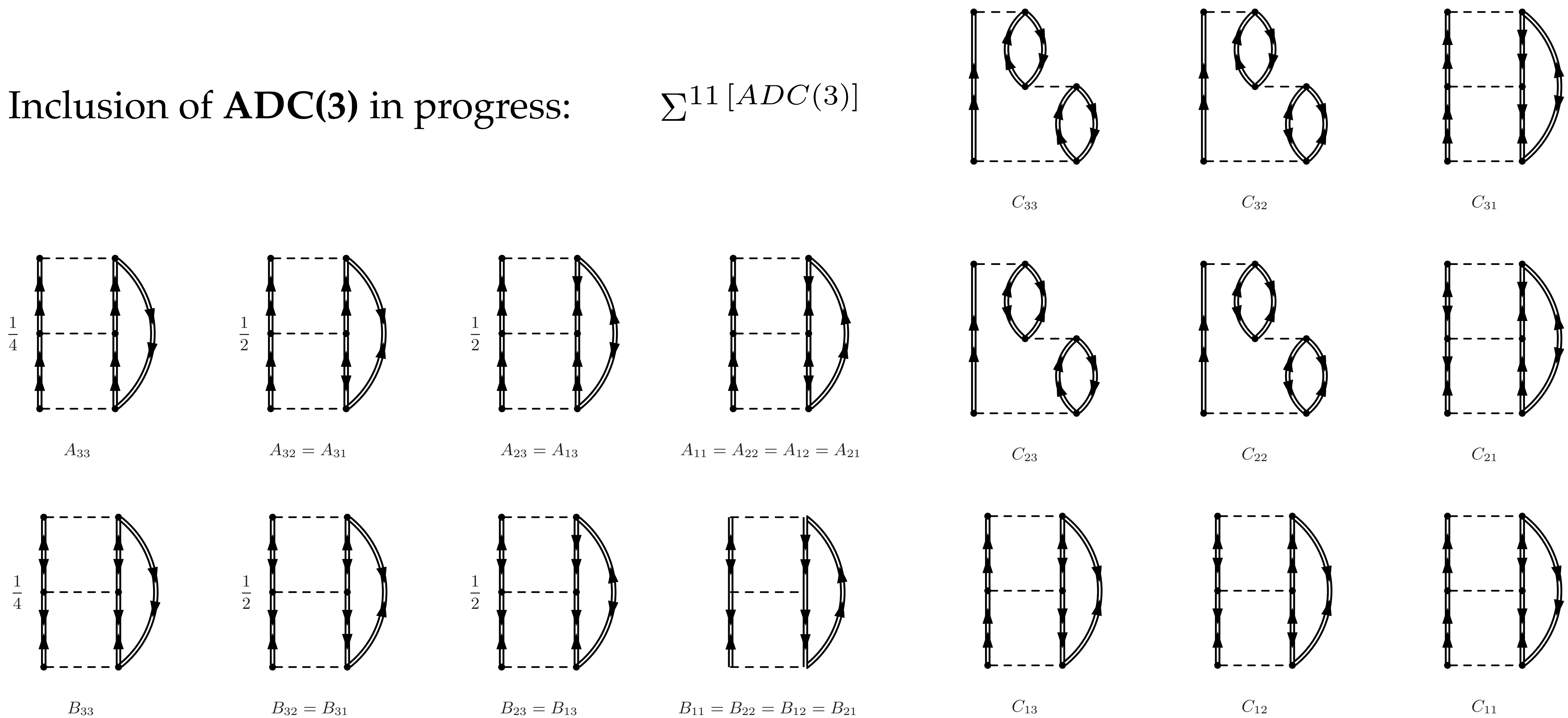


Gorkov-Green's functions

Inclusion of **ADC(3)** in progress: $\Sigma^{11\,[ADC(3)]}$



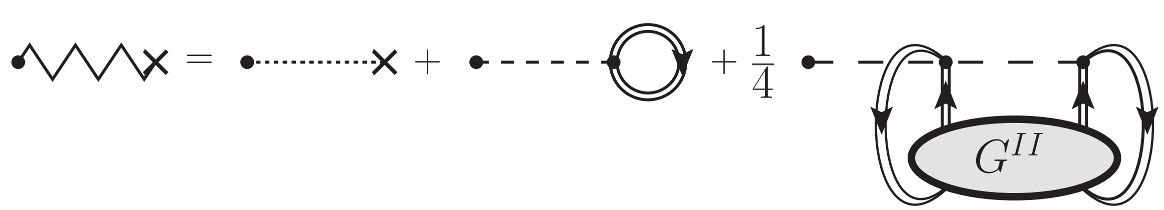
[Barbieri, Duguet & Somà *in prep.*]

ADC(n) diagrams	***n*=1**	**2**	**3**
Dyson	1	1	2
Gorkov	2	4	**34**

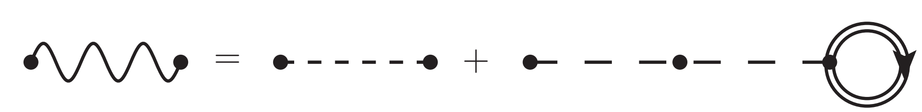
Three-body forces

- Hamiltonians for A-nucleon systems contain in principle up to A-body operators
  - At least **three-body forces** need to be included in realistic ab initio calculations
- Diagrammatic expansion can be simplified by exploiting the concept of **effective interactions**
  - Generalisation of normal ordering (fully correlated density matrices)

effective 1-body

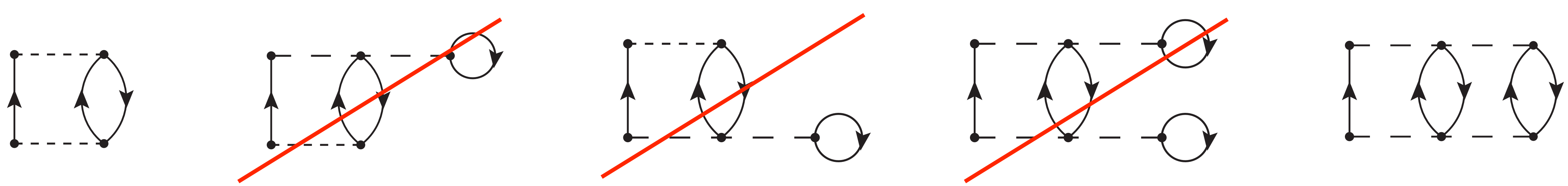


effective 2-body



[Carbone, Cipollone, Barbieri, Rios, Polls 2013]

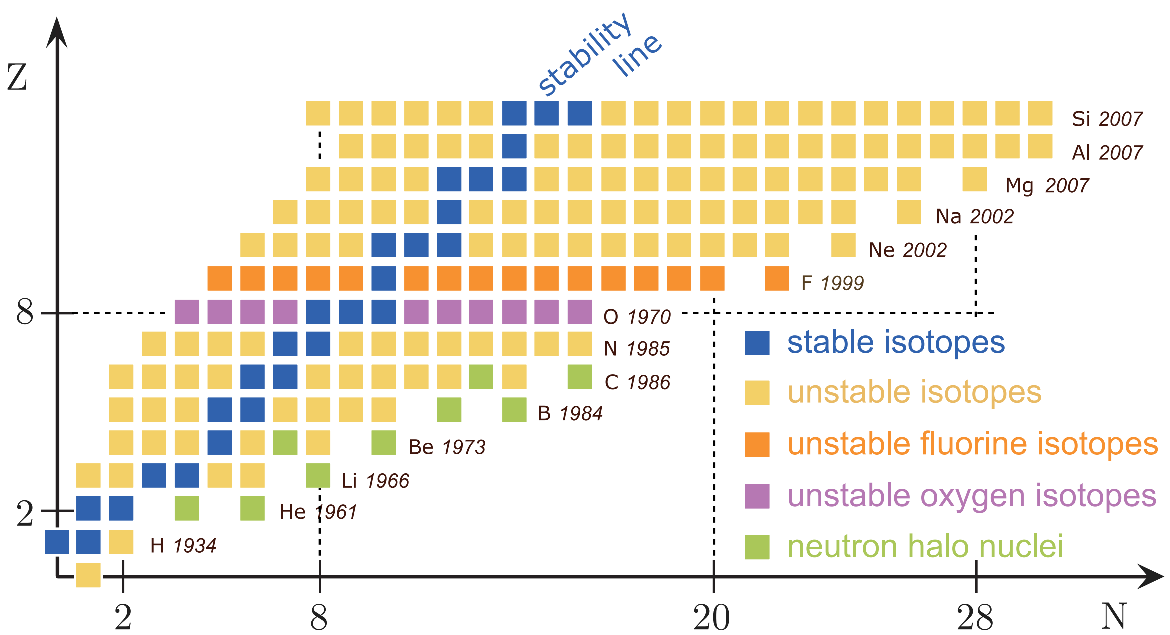
- One introduces **interaction-irreducible** diagrams



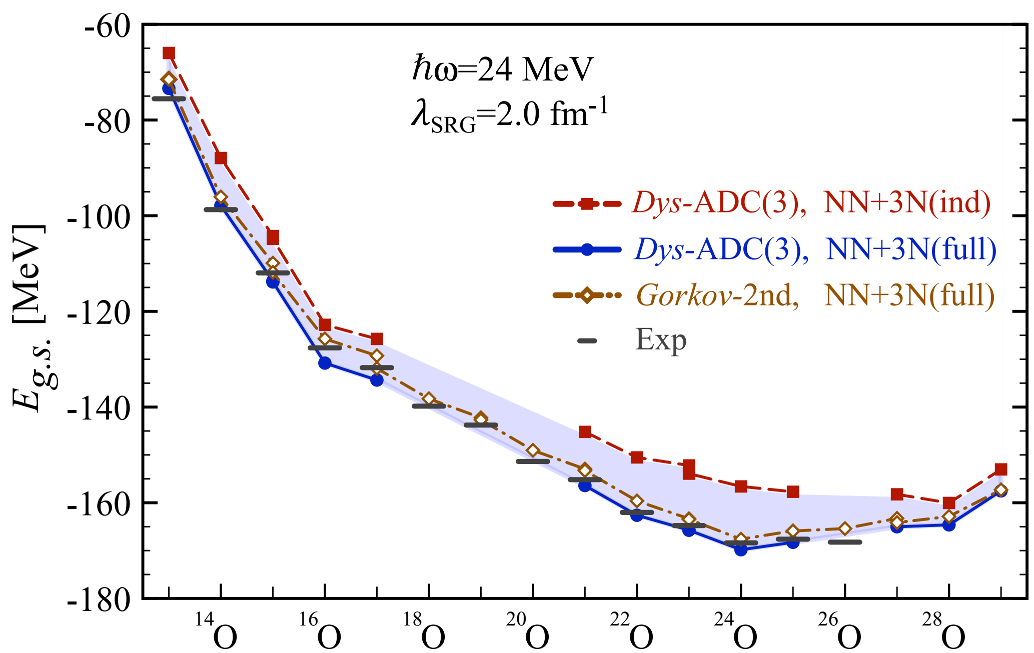
- Galitskii-Migdal-Koltun sum rule needs to be modified to account for 3N term W

$$E_0^N = \frac{1}{2\pi}\int_{-\infty}^{\epsilon_F^-} d\omega \sum_{\alpha\beta}(T_{\alpha\beta}+\omega\delta_{\alpha\beta})\mathrm{Im}\, G_{\beta\alpha}(\omega) - \frac{1}{2}\langle\Psi_0^N|\hat{W}|\Psi_0^N\rangle$$

Oxygen anomaly as ab initio benchmark



Correct reproduction of drip line at ^{24}O



[Cipollone *et al.* 2015]

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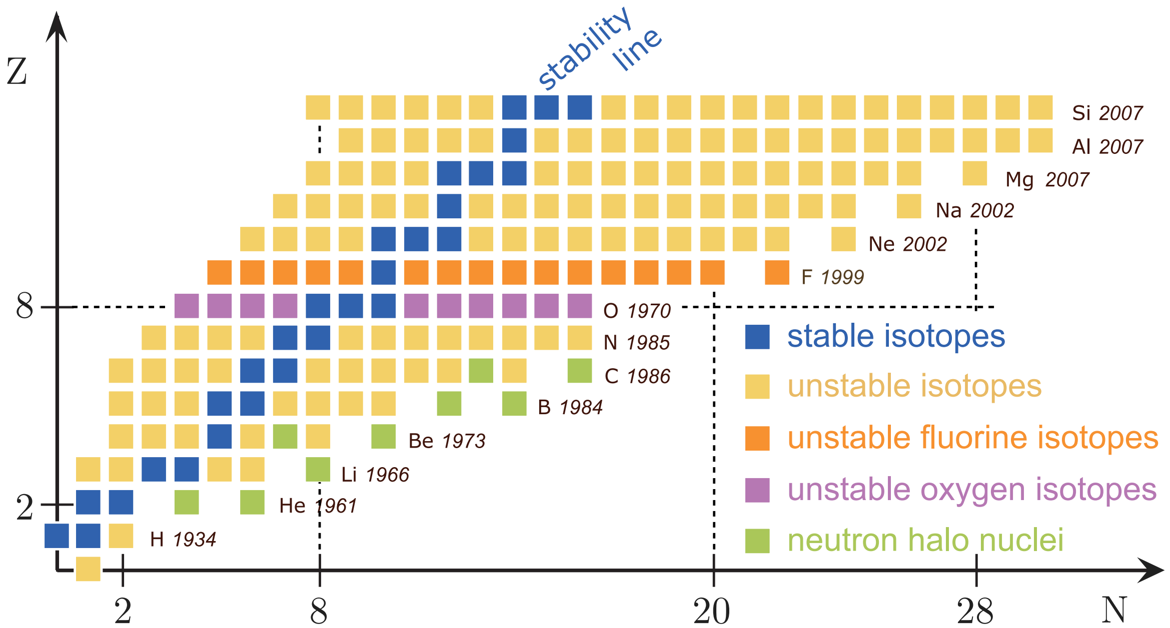

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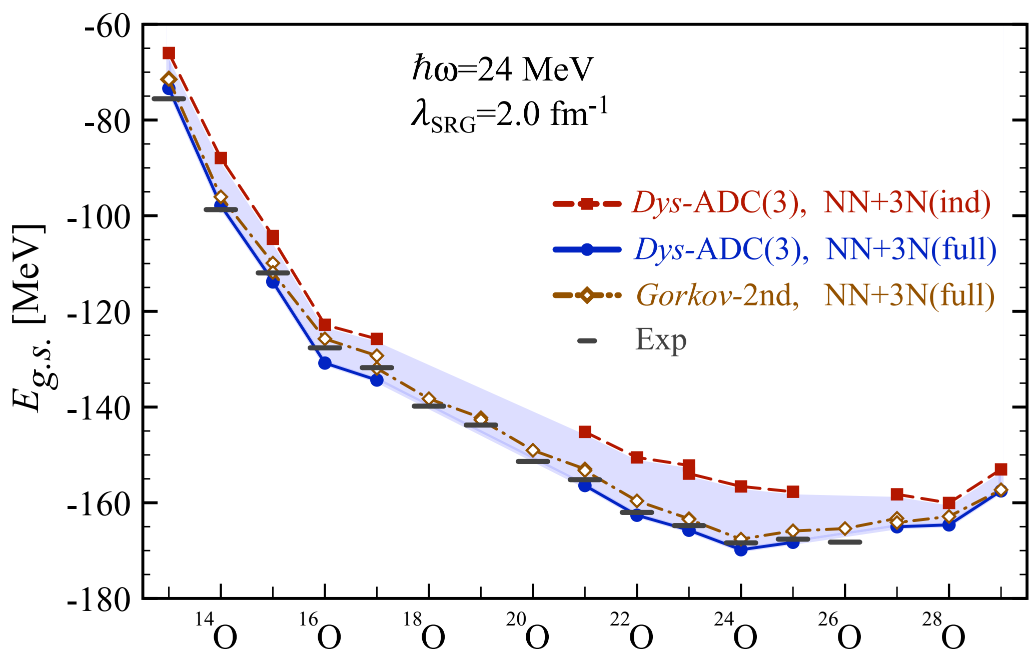
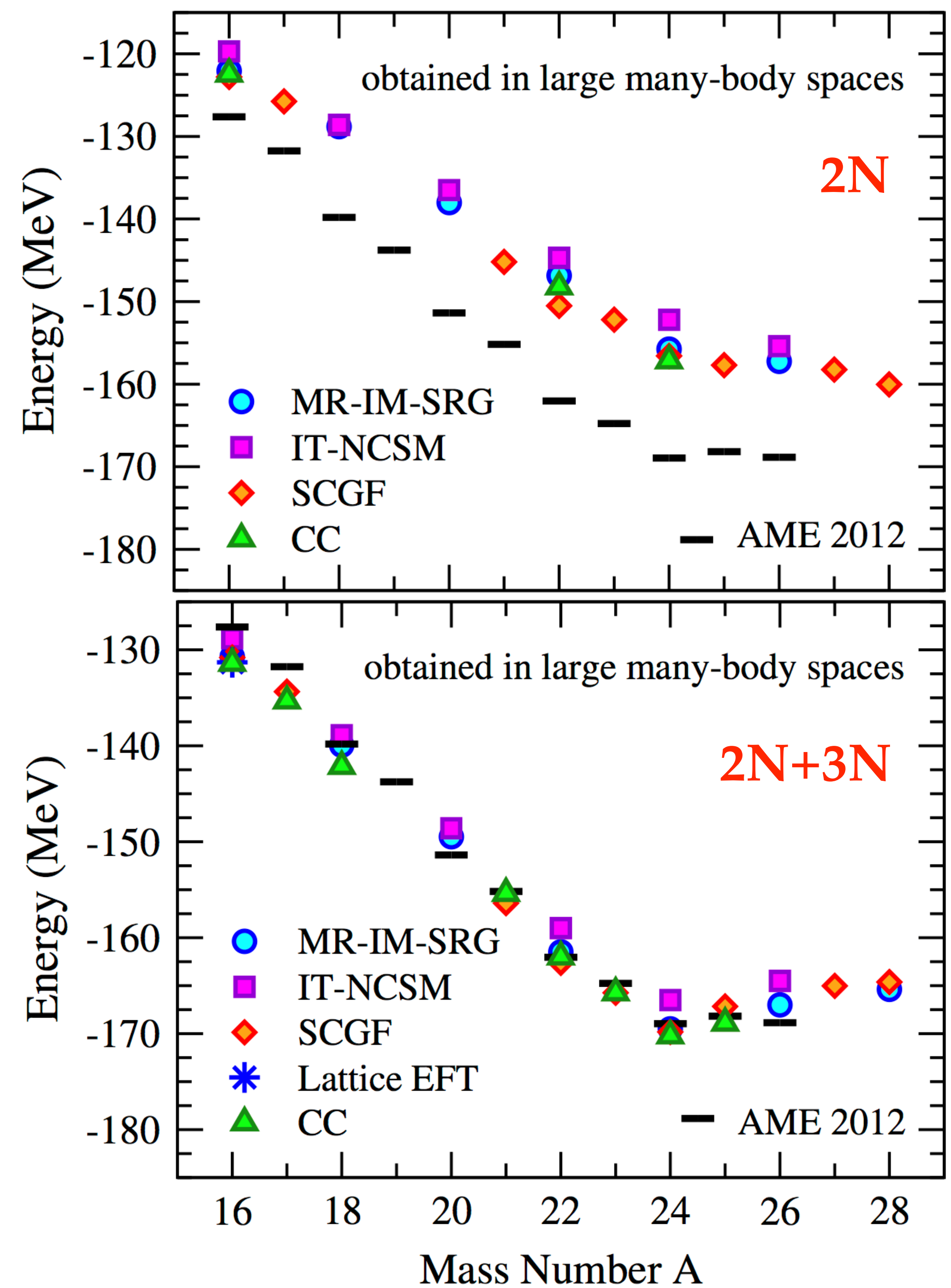


[Cipollone *et al.* 2015]

O chain as testing ground

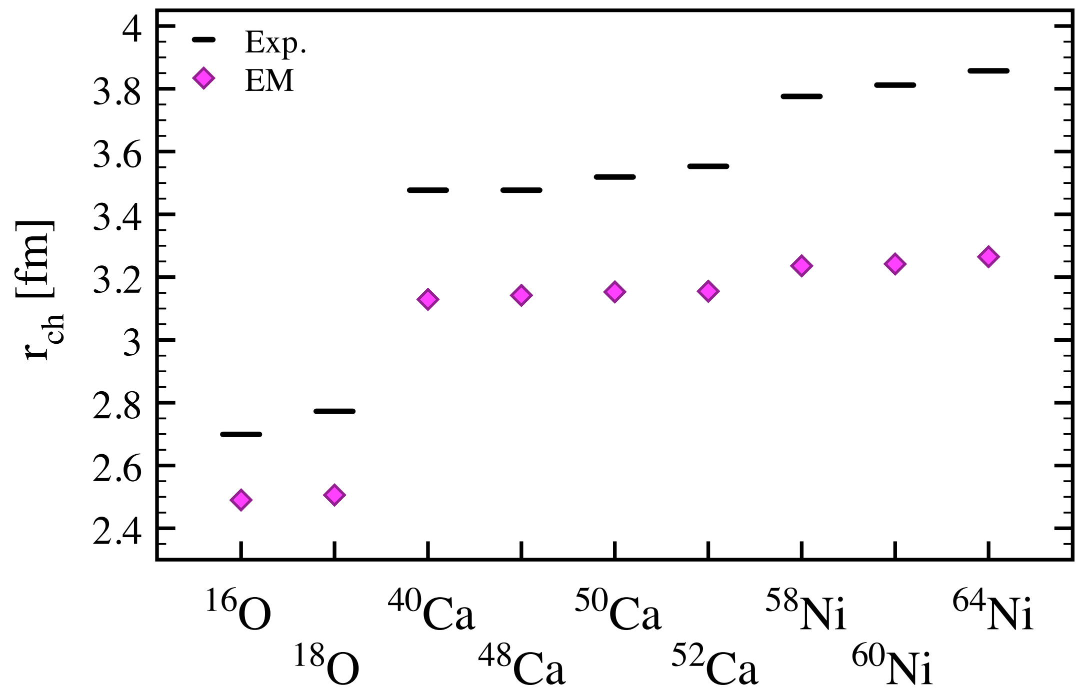


[Hebeler *et al.* 2015]

Changing the strategy: $NNLO_{sat}$

- Standard ChEFT interactions successful in the description of light nuclei

- Description **worsens** when going to heavier systems
  - Spectra too spread out
  - Radii severely underestimated
  - Wrong saturation point of nuclear matter?



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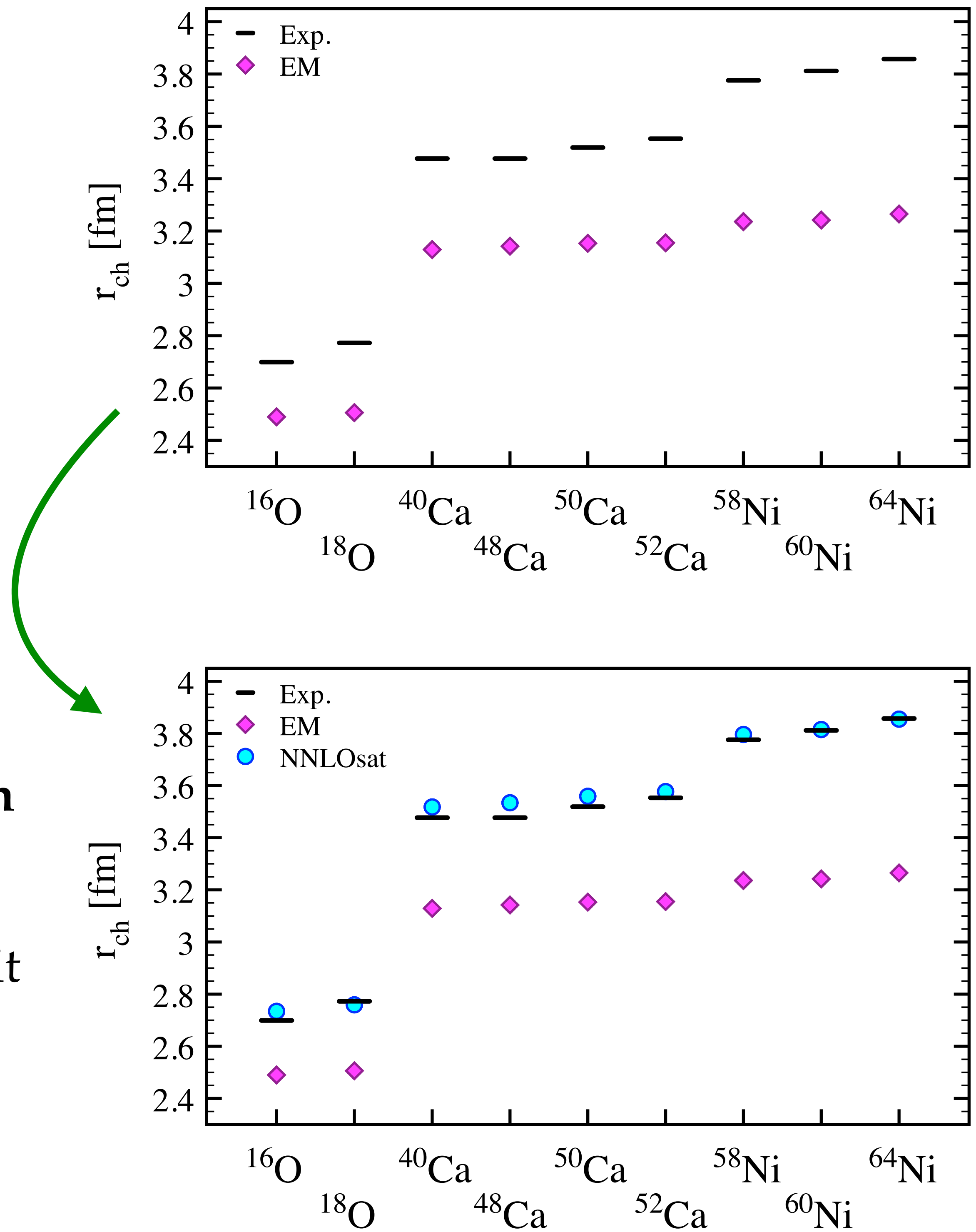
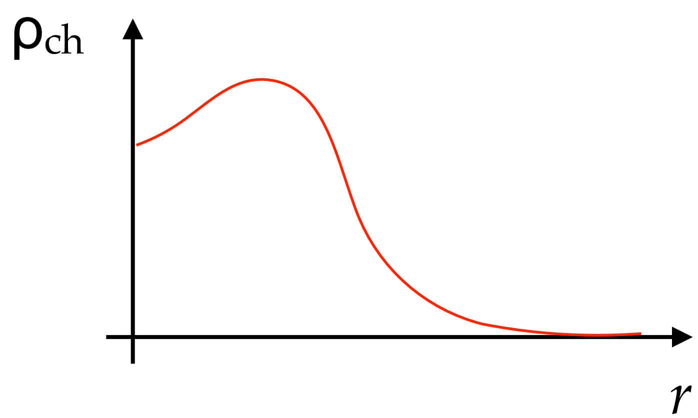


- ⦿ **Prompted the development of $NNLO_{sat}$ Hamiltonian**
  - ○ Simultaneous fit of LEC in 2- and 3-body sectors
  - ○ Data from not-so-light nuclei (A=14-25) included in fit
  - ○ Non-local regulators

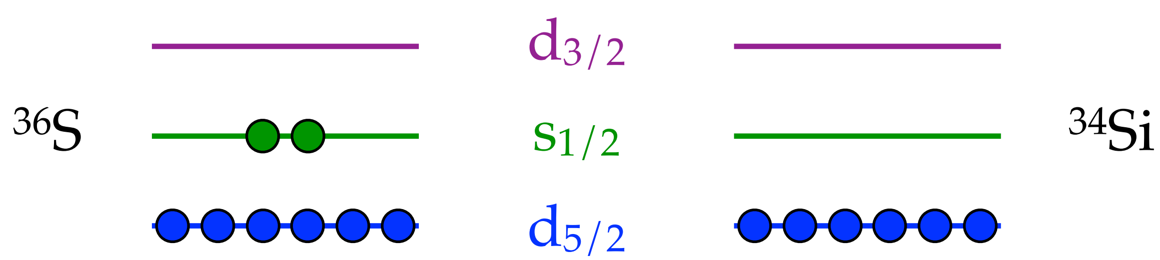
[Ekström *et al*. 2015]

Bubble nuclei?

- **Unconventional depletion** ("bubble") in the centre of ρ_{ch} conjectured for certain nuclei
- **Purely quantum mechanical effect**
  - $\ell = 0$ orbitals display radial distribution peaked at $r = 0$
  - $\ell \neq 0$ orbitals are instead suppressed at small r
  - Vacancy of s states ($\ell = 0$) embedded in larger-ℓ orbitals might cause central depletion
- **Conjectured associated effect on spin-orbit splitting**
  - Non-zero derivative at the interior
  - Spin-orbit potential of "non-natural" sign
  - Reduction of (energy) splitting of low-ℓ spin-orbit partners



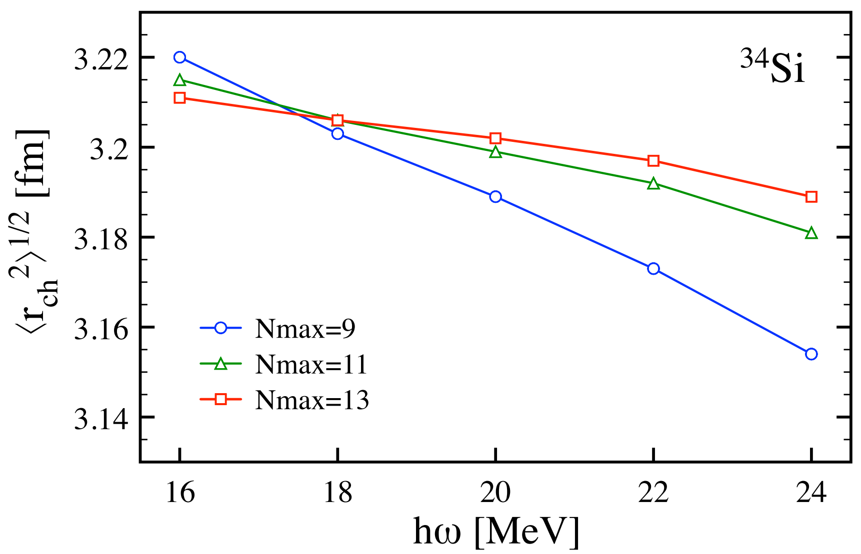
- Bubbles predicted for hyper-heavy nuclei [Dechargé *et al.* 2003]
- In light/medium-mass nuclei the **most promising candidate is ^{34}Si** [Grasso *et al.* 2009, …]

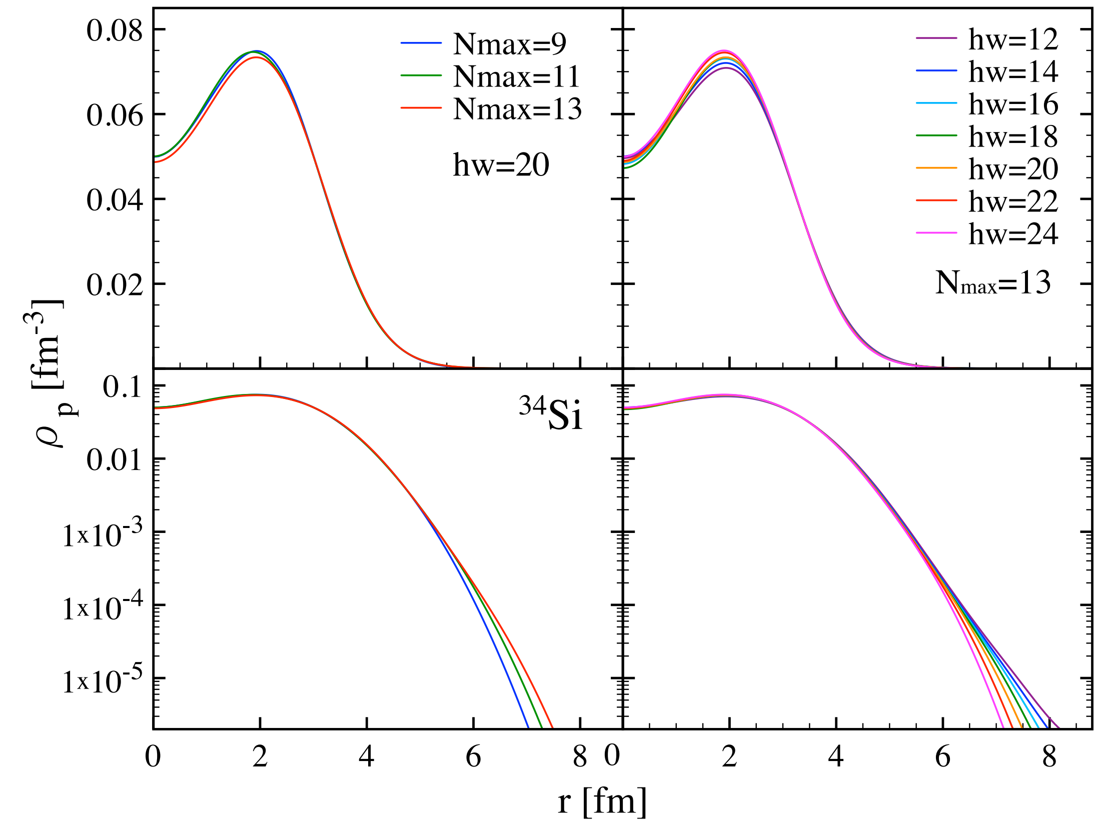


Convergence of the method

- Calculations performed within different many-body truncations [Duguet *et al.* 2017]
  - ADC(1) = HF, ADC(2) & ADC(3)

- **Model space convergence**





- **Many-body convergence**

Binding energies

E [MeV]	ADC(1)	ADC(2)	ADC(3)	Experiment
^{34}Si	-84.481	-274.626	-282.938	-283.427
^{36}S	-90.007	-296.060	-305.767	-308.714

ADC(3) brings only ~5% additional binding

Charge radii

$\langle r_{ch}^2 \rangle^{1/2}$	ADC(1)	ADC(2)	ADC(3)	Experiment
^{34}Si	3.270	3.189	3.187	-
^{36}S	3.395	3.291	3.285	3.2985 ± 0.0024

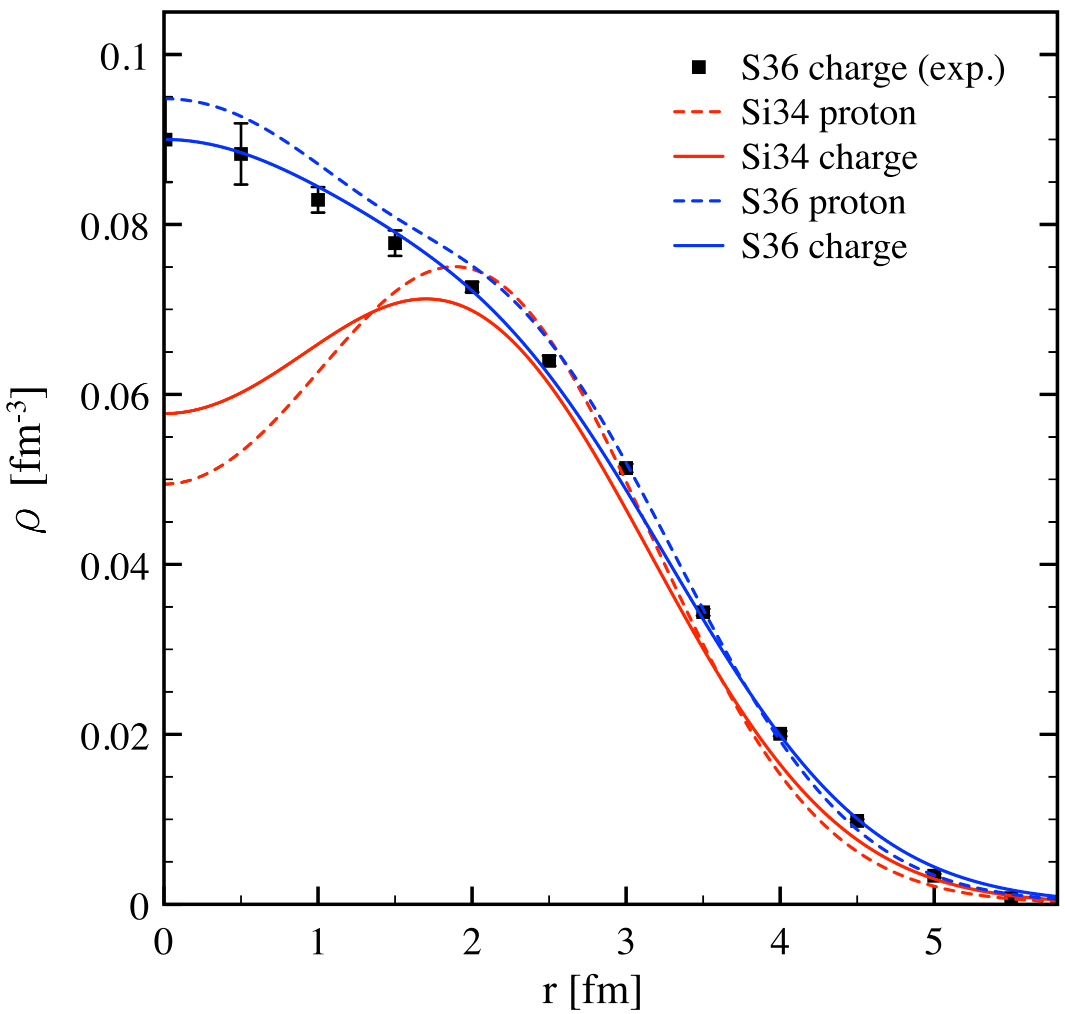
Radii converged already at ADC(2) level

Charge density distribution

⦿ Charge density computed through folding with the finite charge of the proton

$$\rho_{\rm ch}(r) = \sum_{i=1}^{3} \frac{\theta_i}{r_i\sqrt{\pi}} \int_0^{+\infty} dr' \frac{r'}{r} \rho_{\rm p}(r') \left[{\rm e}^{-\left(\frac{r-r'}{r_i}\right)^2} - {\rm e}^{-\left(\frac{r+r'}{r_i}\right)^2} \right]$$

(θ_i, r_i) fitted to reproduce proton charge form factor from e[-] scattering



^{34}Si	SCGF	SCGF*	SREDF [8]	MREDF [9]	MREDF [10]	SM [8]
F_p	0.34	0.34	0.38	0.21	0.22	0.41
$F_{\rm ch}$	0.15	0.19*	0.23	0.09	0.11	0.28

$$F \equiv \frac{\rho_{\rm max} - \rho_{\rm c}}{\rho_{\rm max}}$$

[8] [Grasso *et al.* 2009]

[9] [Yao *et al.* 2012]

[10] [Yao *et al.* 2013]

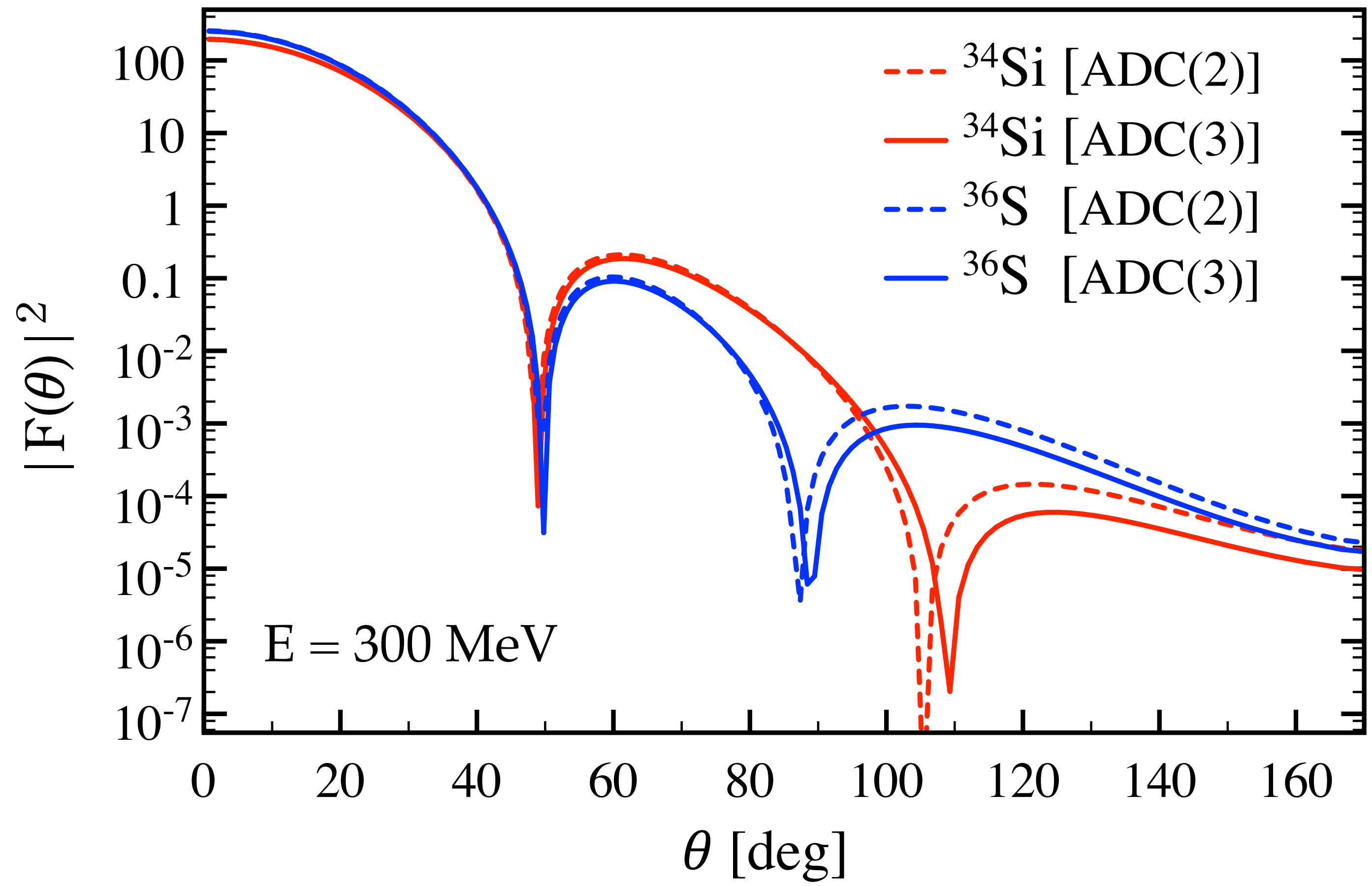
○ Excellent agreement with experimental charge distribution of ^{36}S [Rychel *et al.* 1983]

○ Folding smears out central depletion ➟ **smaller depletion factor** (cf. EDF calculations)

Charge form factor

⊙ Charge form factor measured in (e,e) experiments sensitive to bubble structure?

$$F(q) = \int d\vec{r} \rho_{\mathrm{ch}}(r) e^{-i\vec{q}\cdot\vec{r}} \quad \text{and} \quad q = 2p \sin\theta/2$$



○ Central depletion reflects in larger F(θ) for angles θ>70° and shifted 2$^{\text{nd}}$ minimum

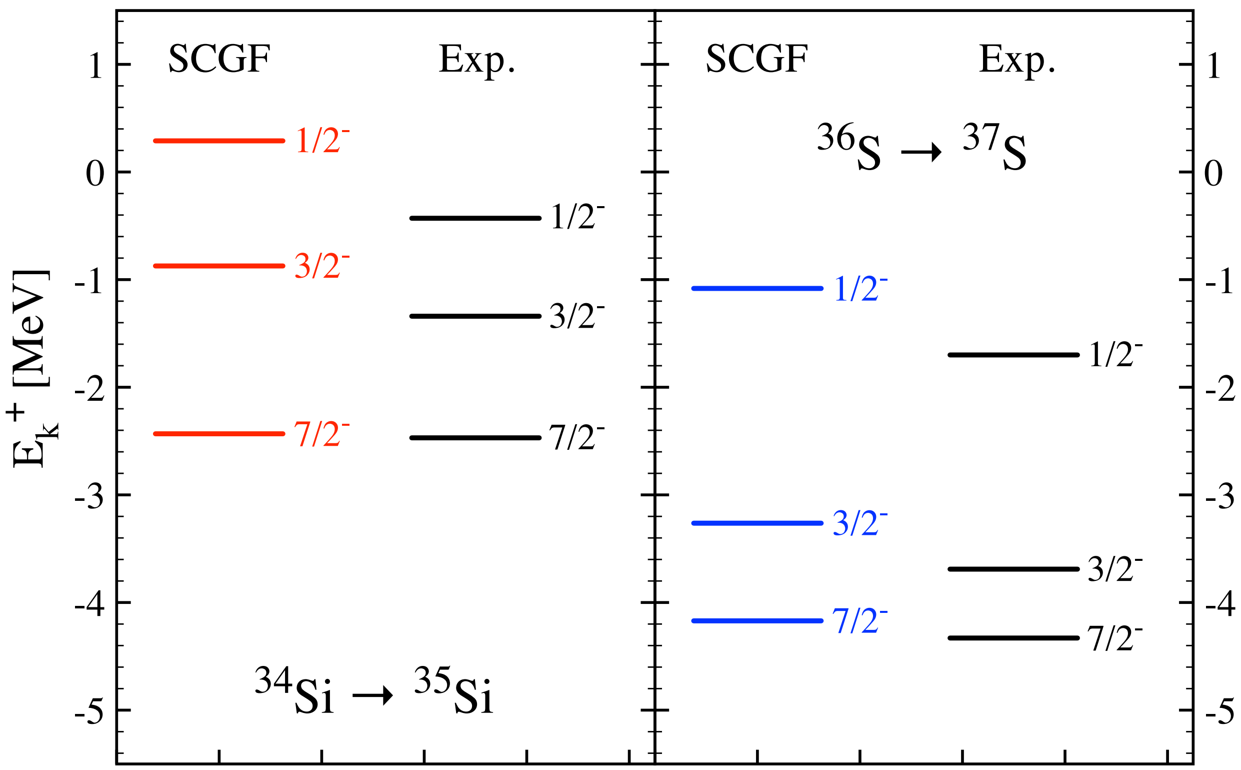
○ **Future electron scattering experiments might be able to see its fingerprints**

Spectroscopy

⦿ Addition and removal spectra compared to **transfer** and **knock-out reactions**

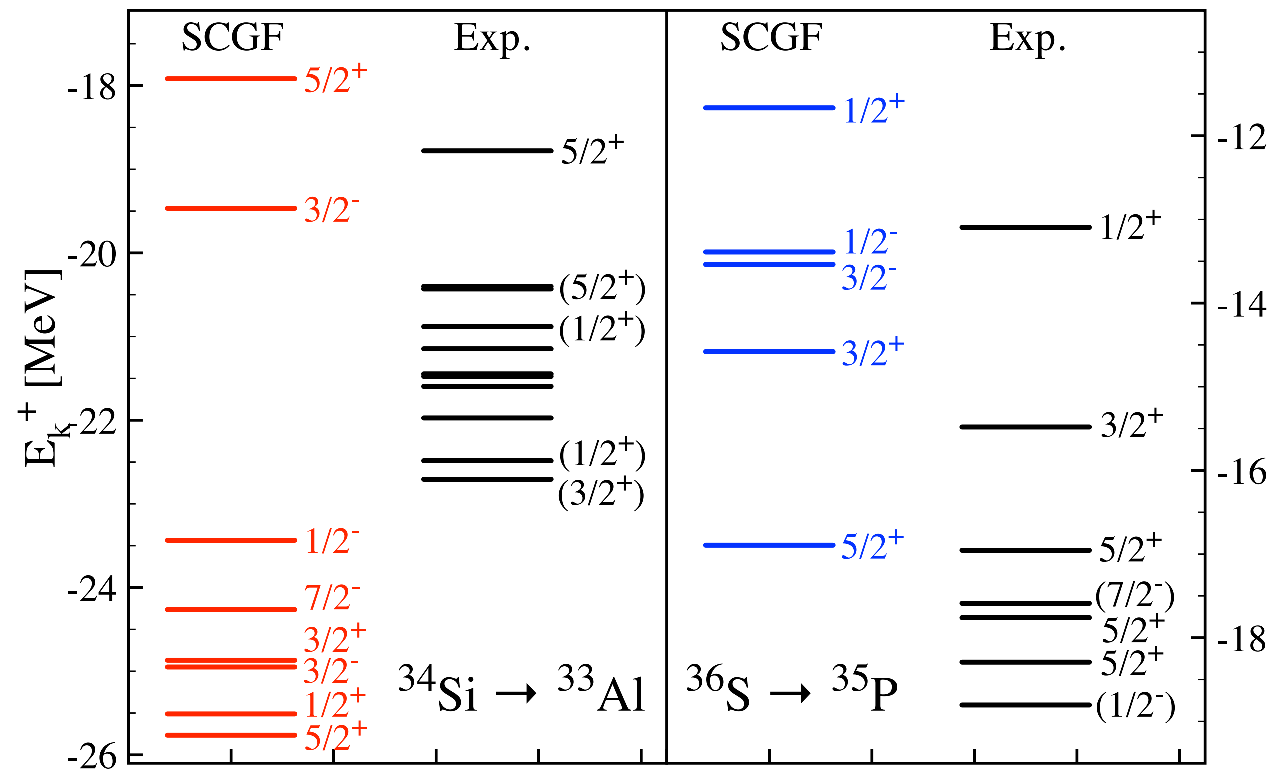
One-neutron addition

Exp. data: [Thorn *et al.* 1984]
[Eckle *et al.* 1989]
[Burgunder *et al.* 2014]



One-proton knock-out

Exp. data: [Khan *et al.* 1985]
[Mutschler *et al.* 2016 (PRC)]
[Mutschler *et al.* 2016 (Nature Phys.)]



○ Good agreement for one-neutron addition, to a lesser extent for one-proton removal

○ **Reduction of $E_{1/2^-}$ - $E_{3/2^-}$ spin-orbit splitting (unique in the nuclear chart!) well reproduced**

Conclusions

⊙ **Many-body formalism well grounded**

- Closed- & open-shell nuclei, g.s. observables & spectroscopy, …
- Two-body propagators to be implemented to access spectroscopy of even-even systems
- Symmetry-restored Gorkov theory?

⊙ **At present, interactions constitute main source of uncertainty**

- ChEFT is undergoing intense development, facing fundamental & practical issues
- *Pragmatic* $NNLO_{sat}$ interaction performs well over good range of nuclei & observables

⊙ **Ab initio applications become competitive with other methods**

- Mid-mass region of the nuclear chart being scrutinised
- Example of potential bubble nucleus ^{34}Si

Appendix

Spectral strength distribution

- Bonus: one-body Green's function contains information about ***A*±1 excitation energy spectra**

- **Spectral representation**

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

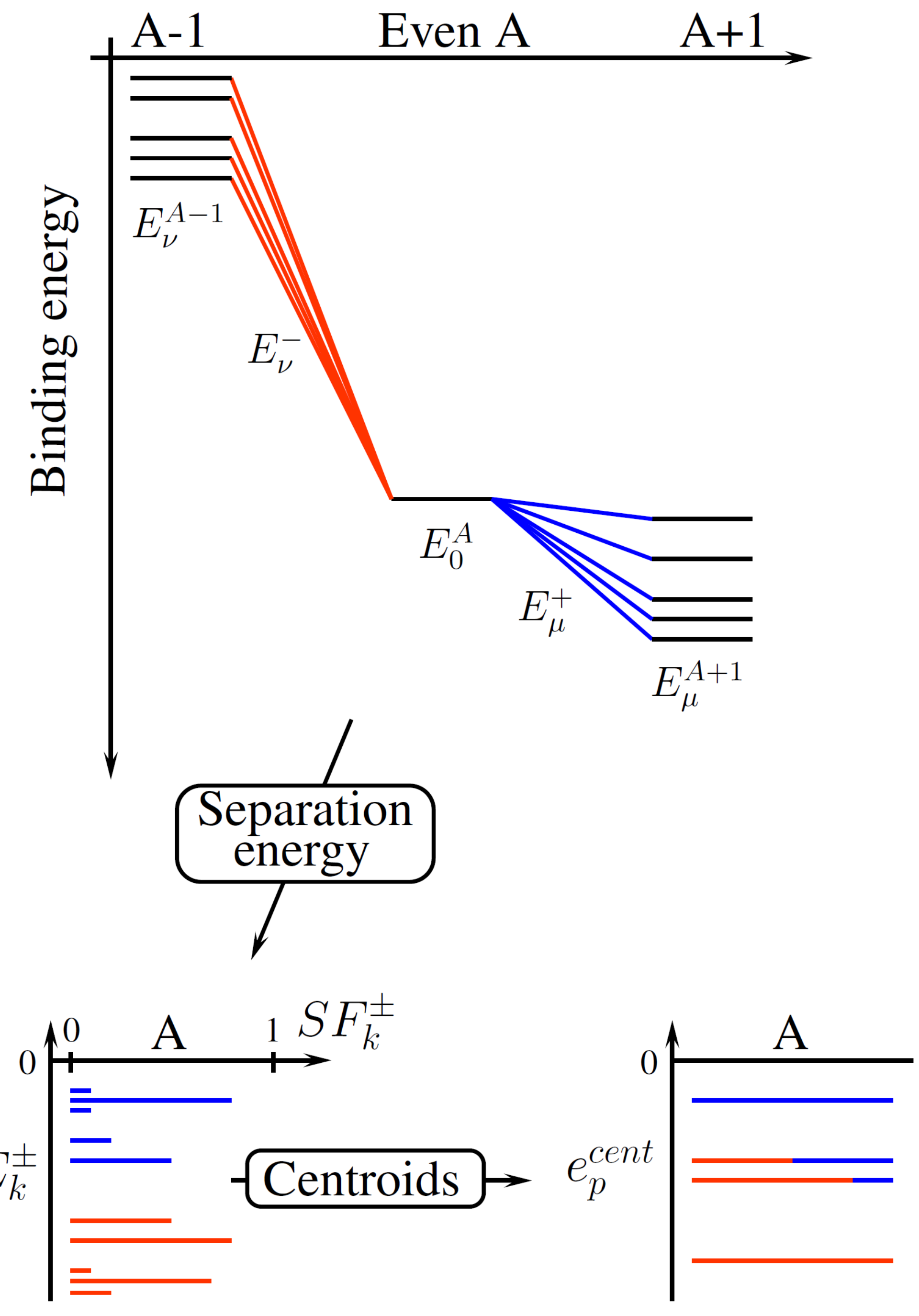
where
$$\begin{cases} \mathcal{U}^{k*}_a \equiv \langle \Psi_k | a^\dagger_a | \Psi_0 \rangle \\ \mathcal{V}^{k*}_a \equiv \langle \Psi_k | \bar{a}_a | \Psi_0 \rangle \end{cases}$$

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**

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

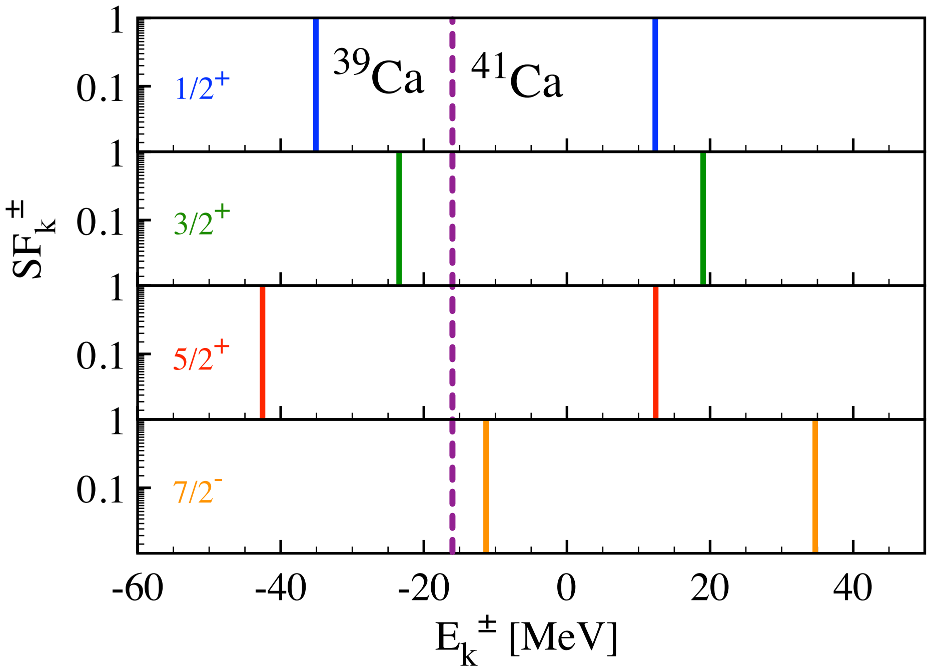
$$SF^-_k \equiv \sum_{a \in \mathcal{H}_1} \left| \langle \psi_k | a_a | \psi_0 \rangle \right|^2 = \sum_{a \in \mathcal{H}_1} \left| \mathcal{V}^k_a \right|^2$$



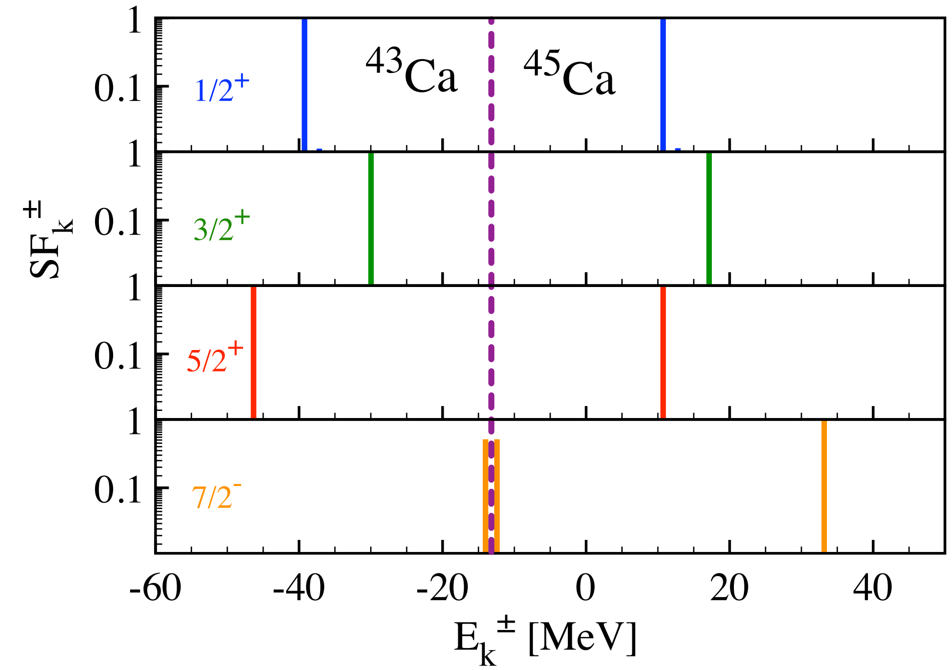
[figure from J. Sadoudi]

Spectral strength distribution: Dyson vs Gorkov

Dyson 1st order (HF)



Gorkov 1st order (HFB)

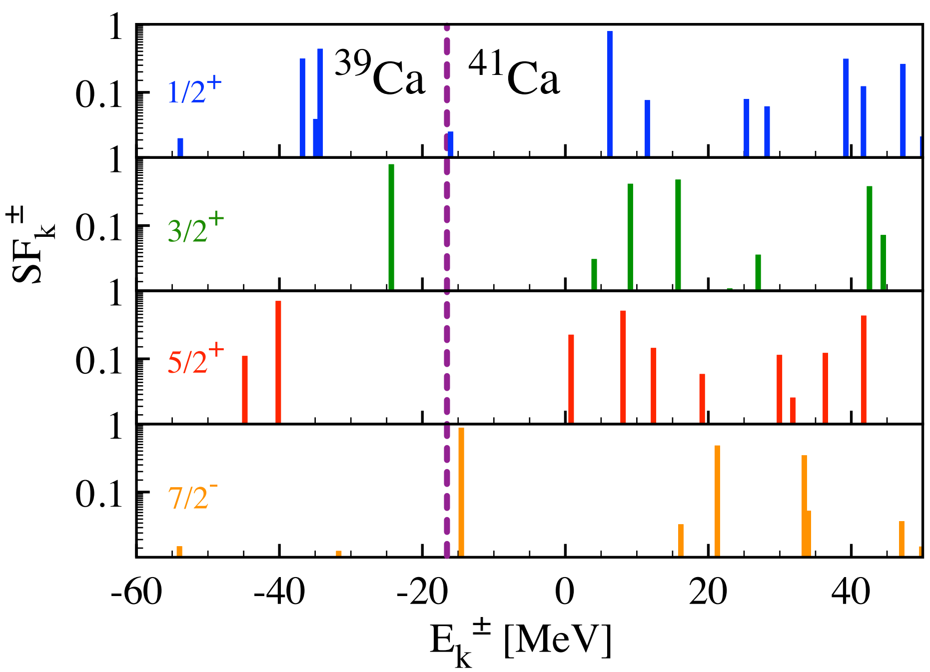


Fragmentation

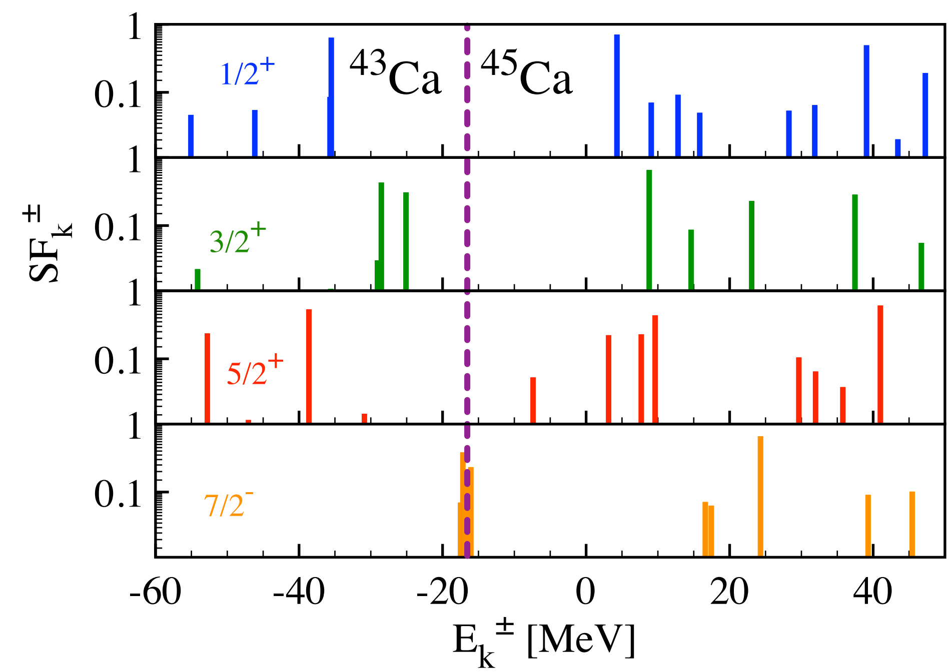
Static pairing

Dynamical fluctuations

Dyson 2nd order

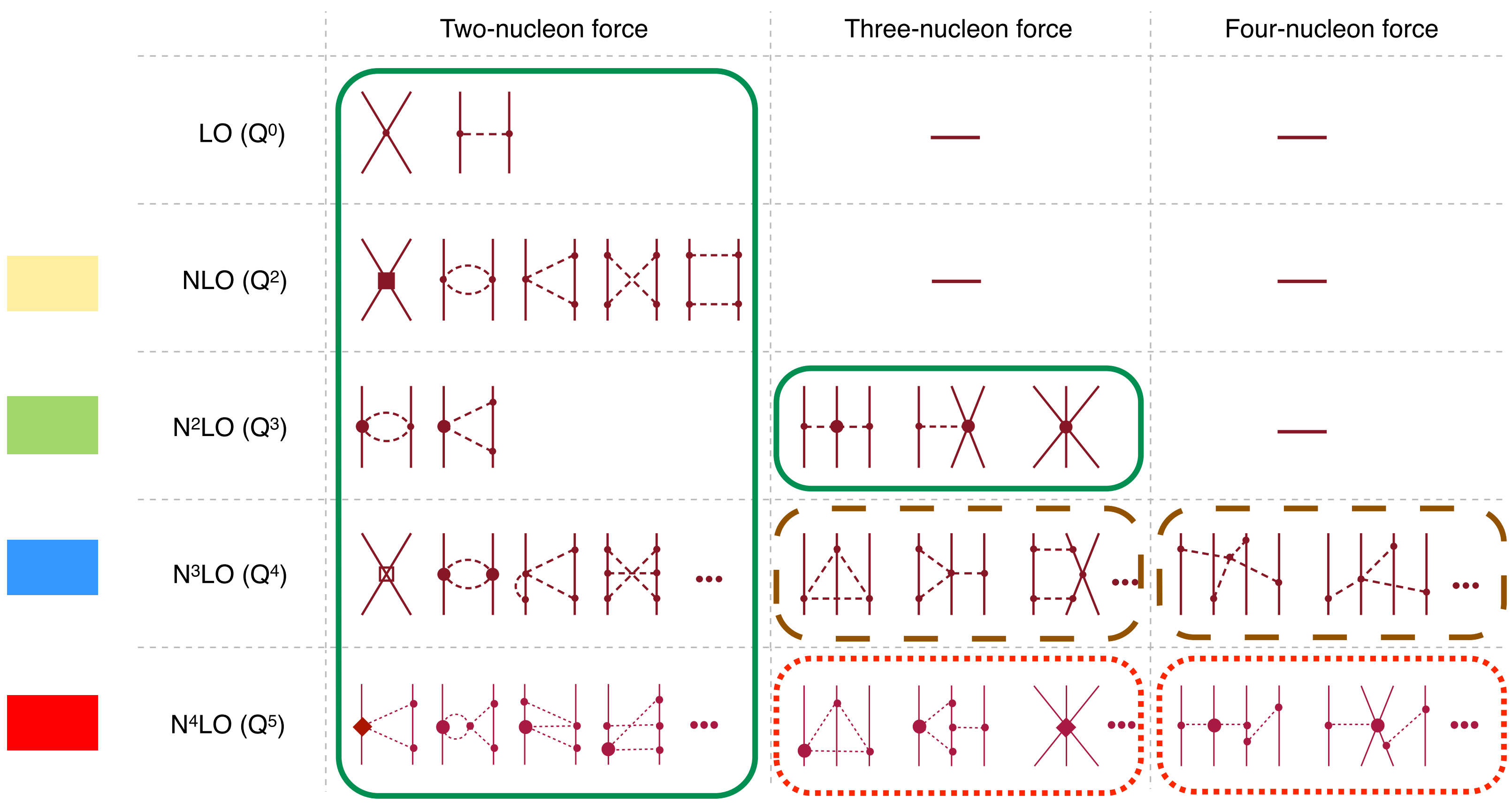


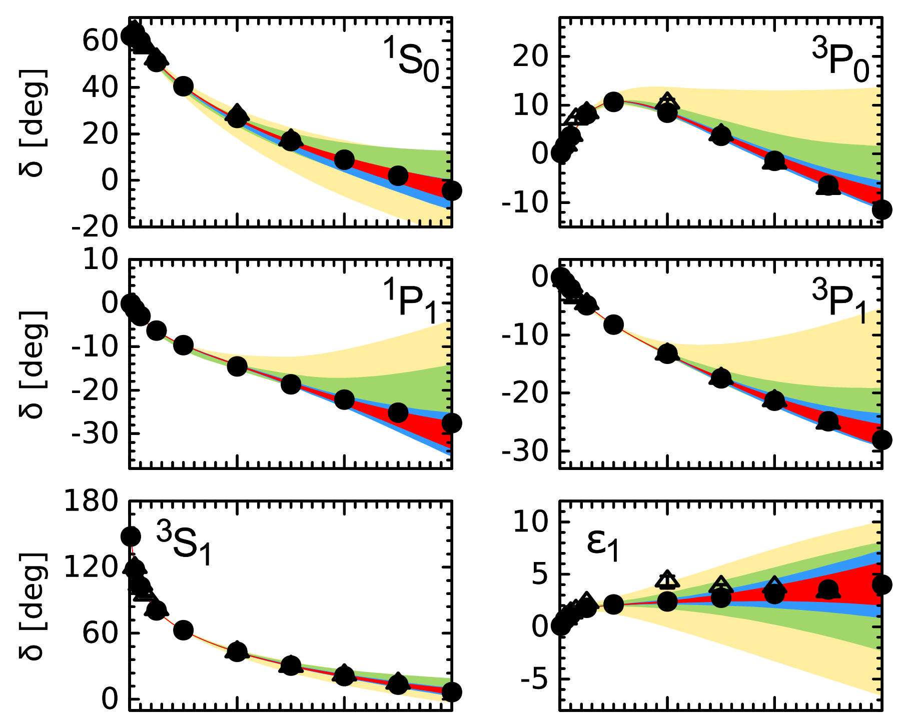
Gorkov 2nd order



Chiral EFT & many-body problem in principle

- **Chiral effective field theory** as a systematic framework to construct *A*N interactions (*A*=2, 3, …)
  - Symmetries of underlying theory built in
  - Hierarchy dictated by power counting
  - Coupling constants fixed by QCD (when possible) or low-energy data
  - One hopes that 2N & 3N (& maybe 4N) forces are sufficient to solve the many-body problem





[Meißner 2016]

- **Ideally**, perform order-by-order many-body calculations with **propagated uncertainties**

Three-body forces

⦿ Galitskii-Migdal-Koltun sum rule needs to be modified to account for 3N term W

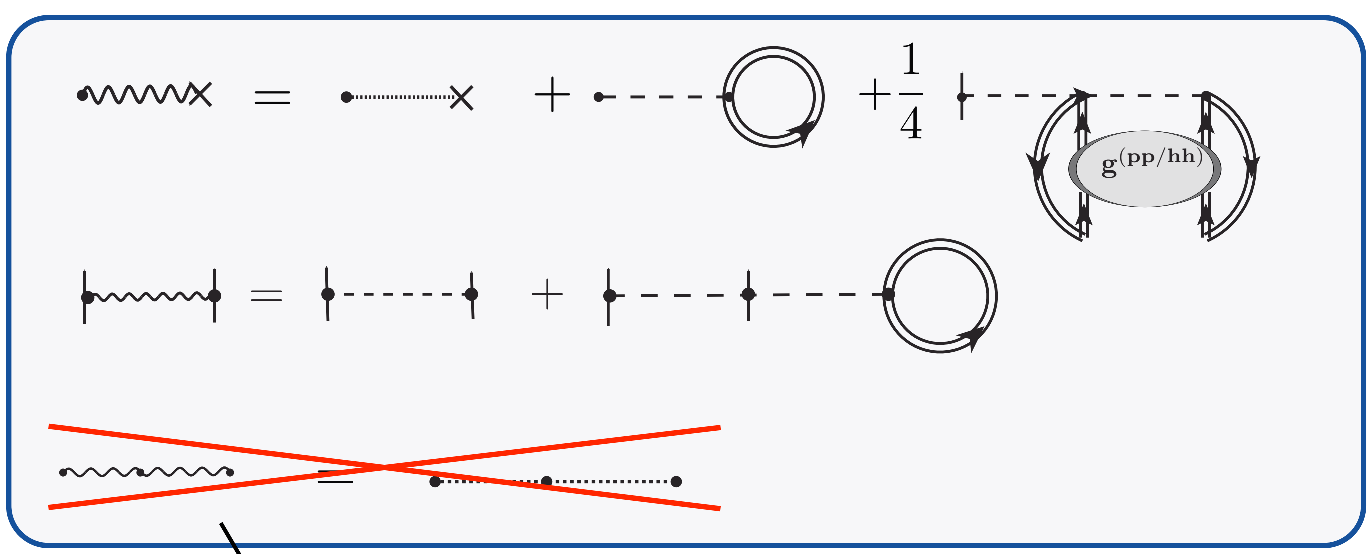
$$E_0^N = \frac{1}{2\pi}\int_{-\infty}^{\epsilon_F^-} d\omega \sum_{\alpha\beta}(T_{\alpha\beta} + \omega\delta_{\alpha\beta})\mathrm{Im}\, G_{\beta\alpha}(\omega) - \frac{1}{2}\langle\Psi_0^N|\hat{W}|\Psi_0^N\rangle$$

[Carbone, Cipollone, Barbieri, Rios, Polls 2013]

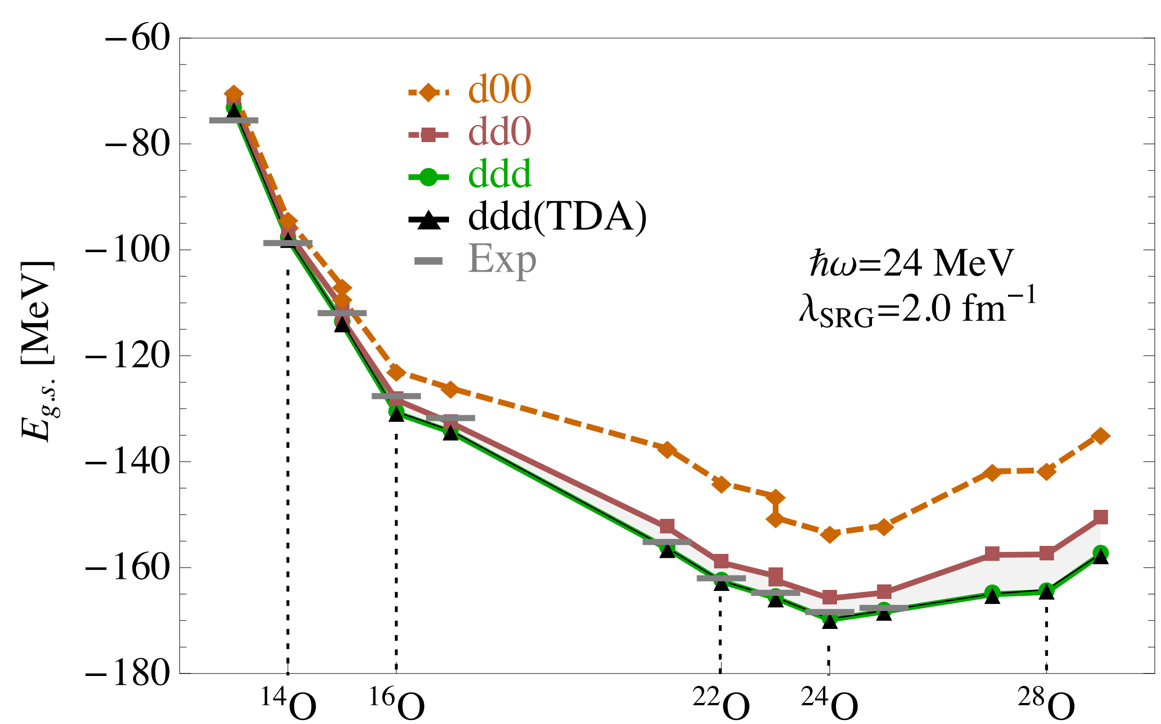
⦿ Effective interactions can be seen as a **generalisation of normal-ordered interactions**

➟ Here contractions are performed with the **fully correlated density matrix**

⦿ Extra correlation provided by the use of dressed propagators can be tested in realistic calculations



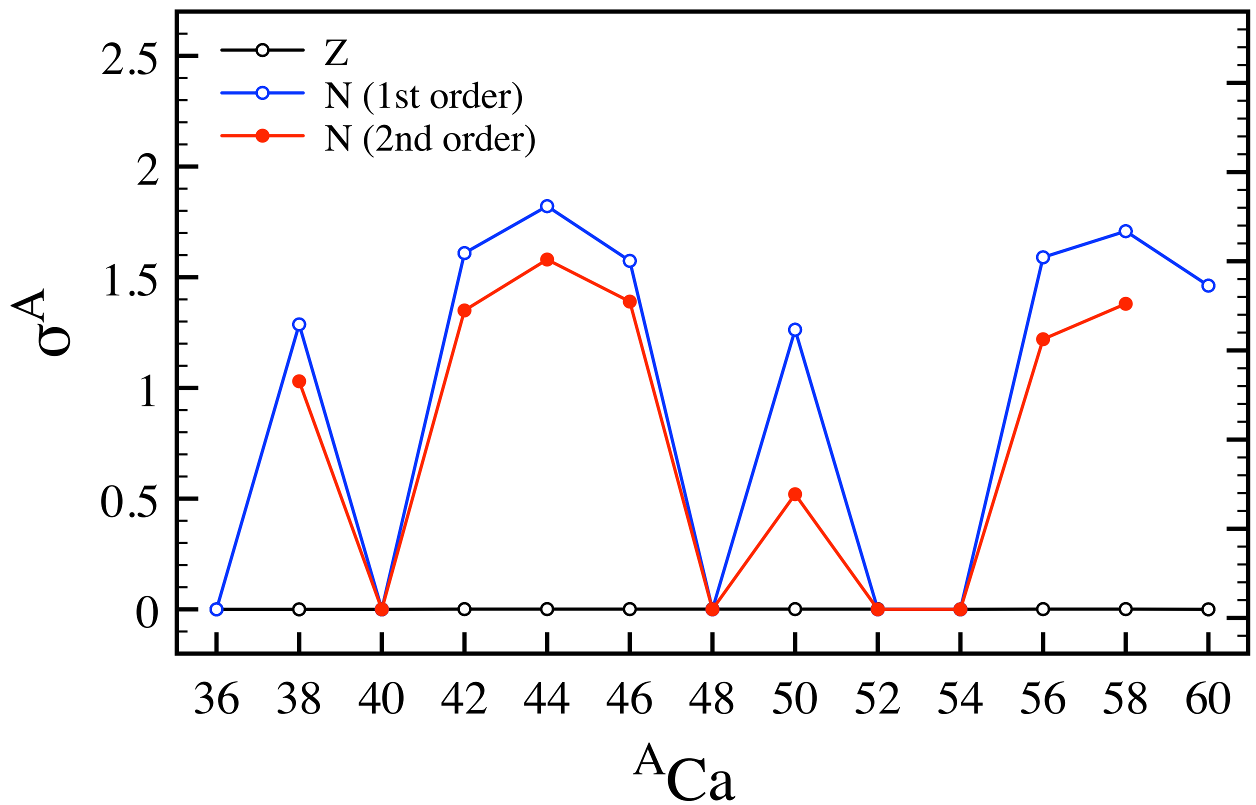
Residual three-body term neglected



[Barbieri *et al.* unpublished]

Symmetry breaking and restoration

⦿ Variance in particle number as an indicator of symmetry breaking



$$\sigma_A = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$$

➟ Only concerns neutron number

➟ Decreases as many-body order increases

⦿ Eventually, symmetries need to be restored

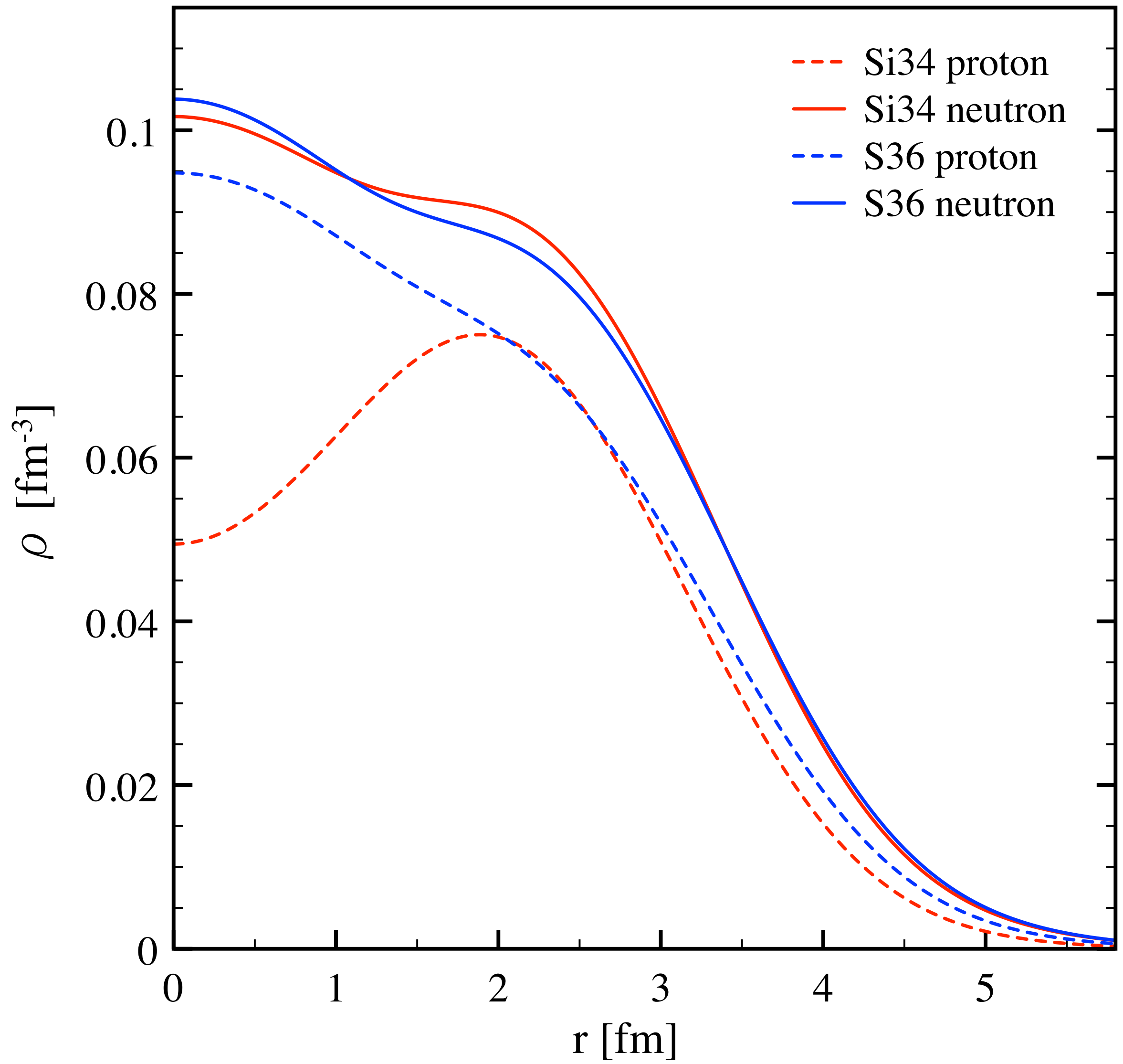
⦿ Only recently the formalism was developed for MBPT and CC

- ○ Case of **SU(2)** [Duguet 2014]
- ○ Case of **U(1)** [Duguet & Signoracci 2016]

⦿ Symmetry-restored Gorkov GF formalism still to be developed

Point-nucleon densities

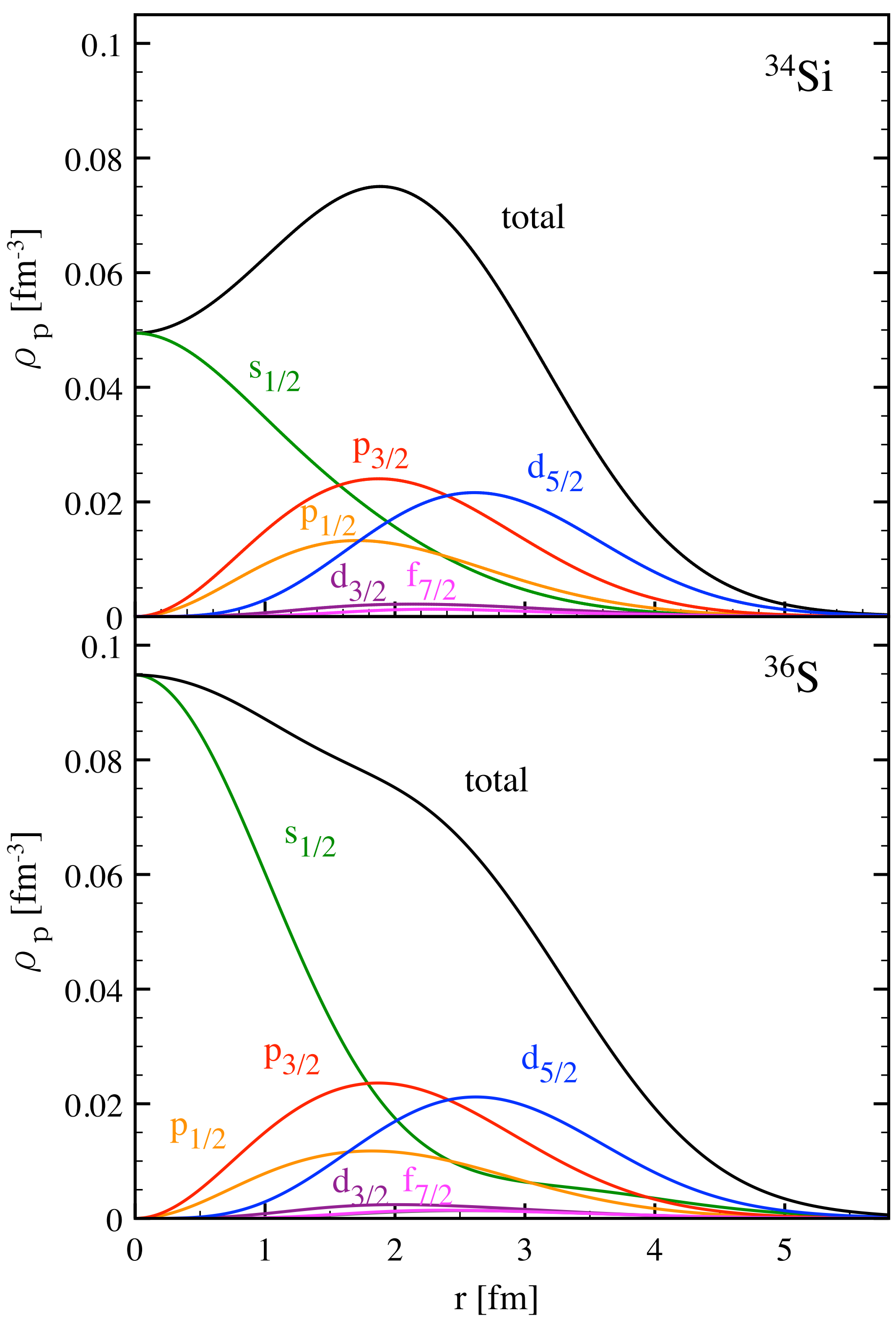
- **Point-proton** density of ^{34}Si displays a marked depletion in the centre
- **Point-neutron** distributions little affected by removal/addition of two protons
- Bubble structure can be quantified by the **depletion factor** $F \equiv \frac{\rho_{\rm max} - \rho_{\rm c}}{\rho_{\rm max}}$ ➟ $F_{\rm p}(^{34}\text{Si}) = 0.34$

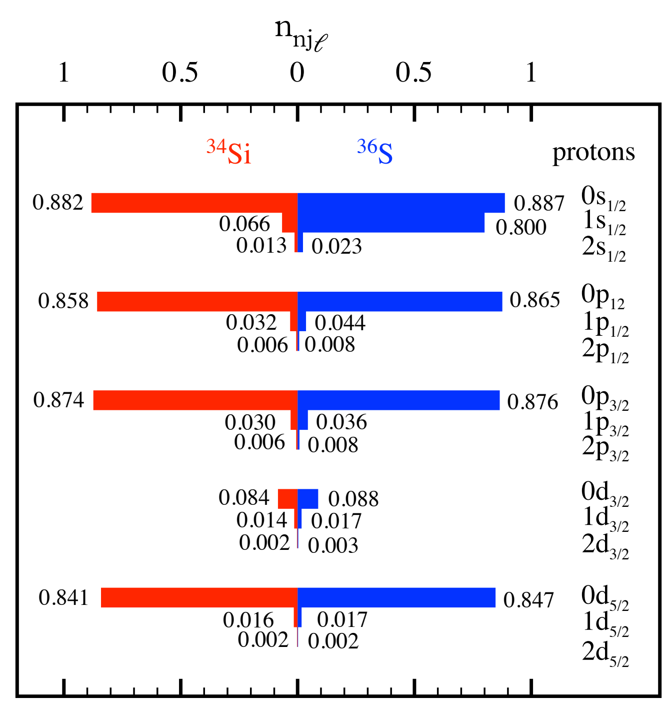


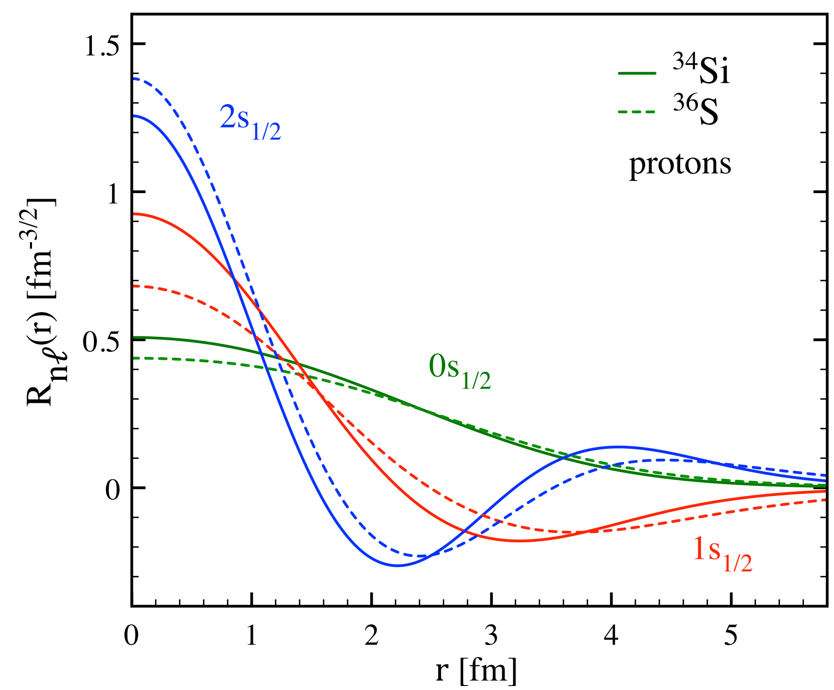
➟ Going from proton to (observable) charge density will smear out depletion

Partial wave decomposition

- Point-proton distributions can be analysed (internally to the theory) in the **natural basis**
- Consider different partial-wave (ℓ, j) contributions $\rho_{\rm p}(\vec{r}) = \sum_{n\ell j} \frac{2j+1}{4\pi} n_{n\ell j} R^2_{n\ell j}(r) \equiv \sum_{\ell j} \rho_{\rm p}^{\ell j}(r)$



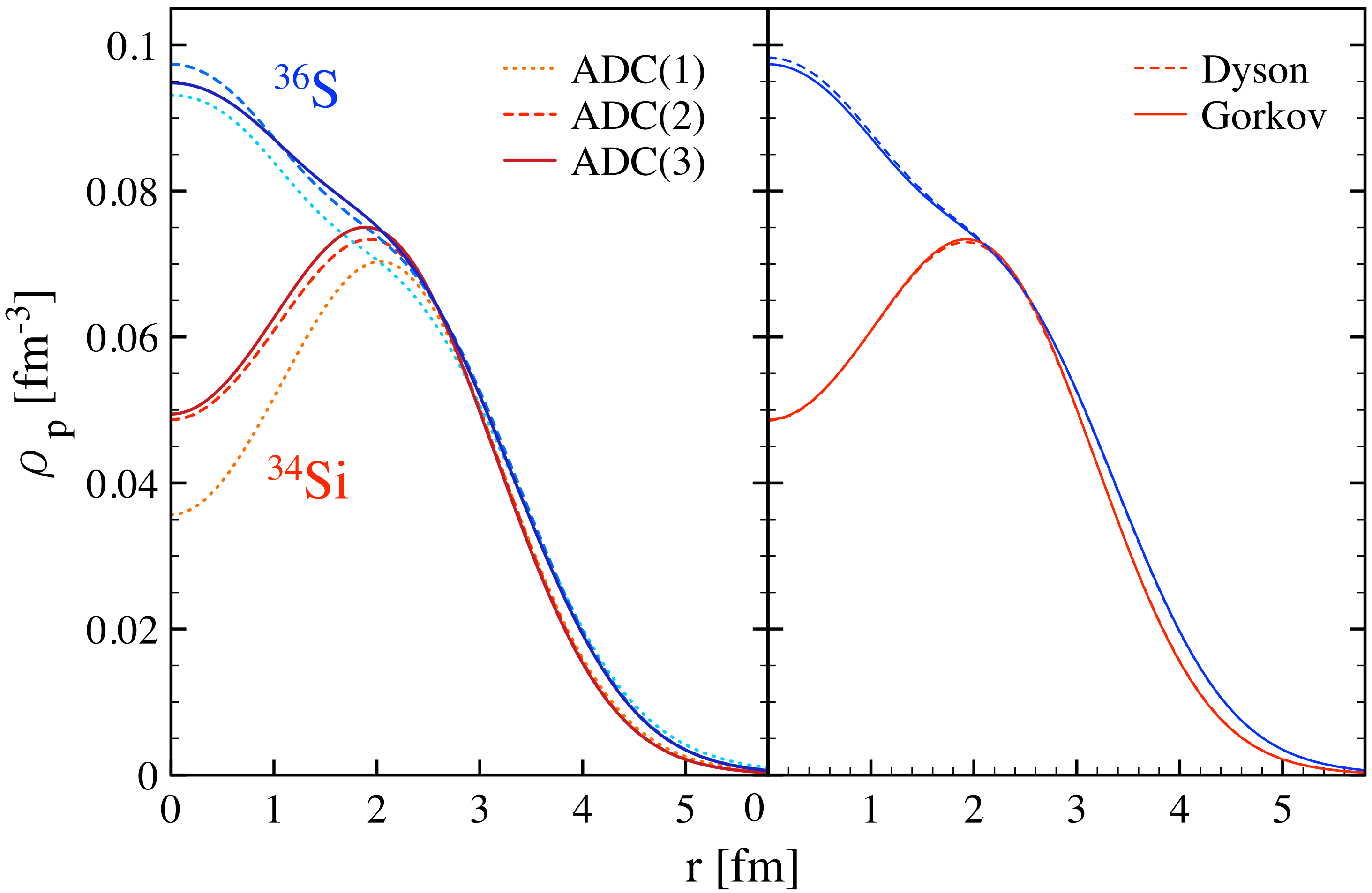


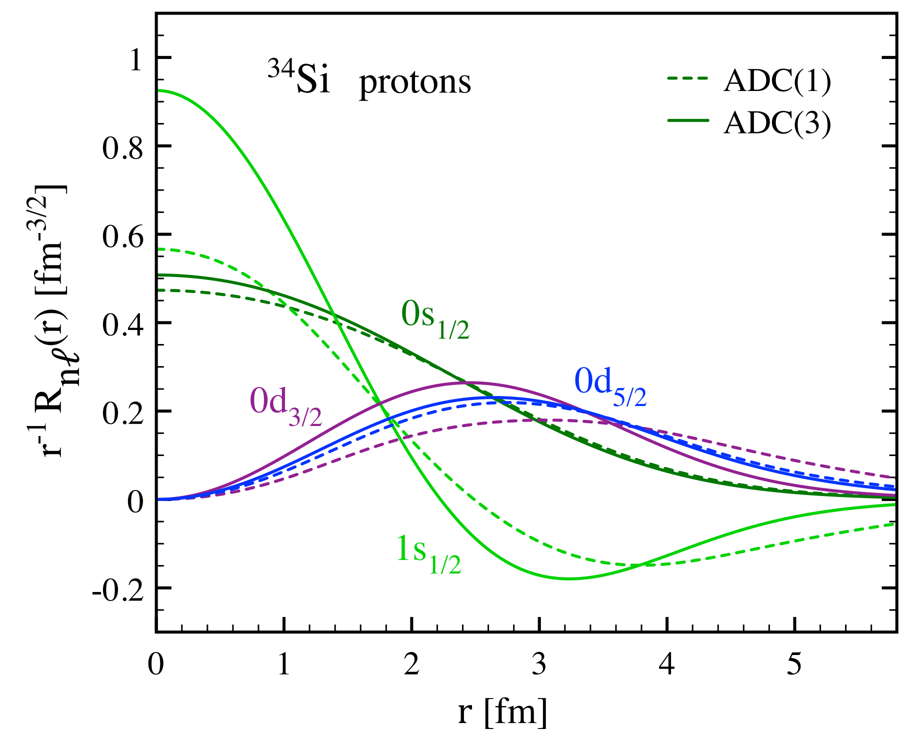


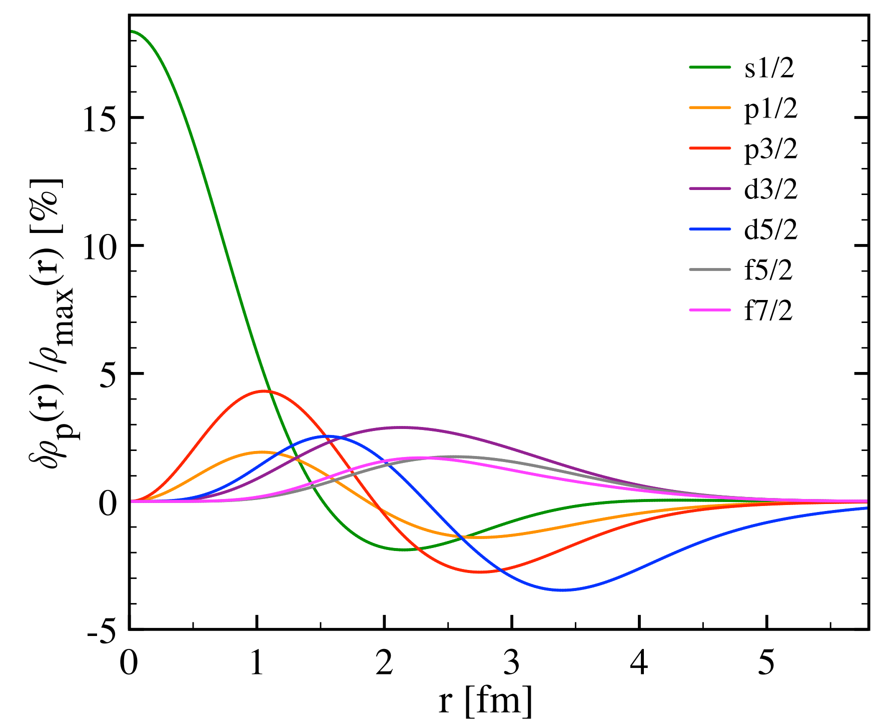
- Independent-particle filling mechanism **qualitatively OK**
- **Quantitatively**, net effect from **balance between n=0, 1, 2**
- Point-neutron contributions & occupations unaffected

Impact of correlations

◉ Impact of correlations analysed by comparing different ADC truncations







○ Dynamical correlations cause **erosion** of the bubble

^{34}Si	ADC(1)	ADC(2)	ADC(3)
F_p	0.49	0.34	0.34

○ Wave functions get contracted ➟ $1s_{1/2}$ peaked at $r = 0$

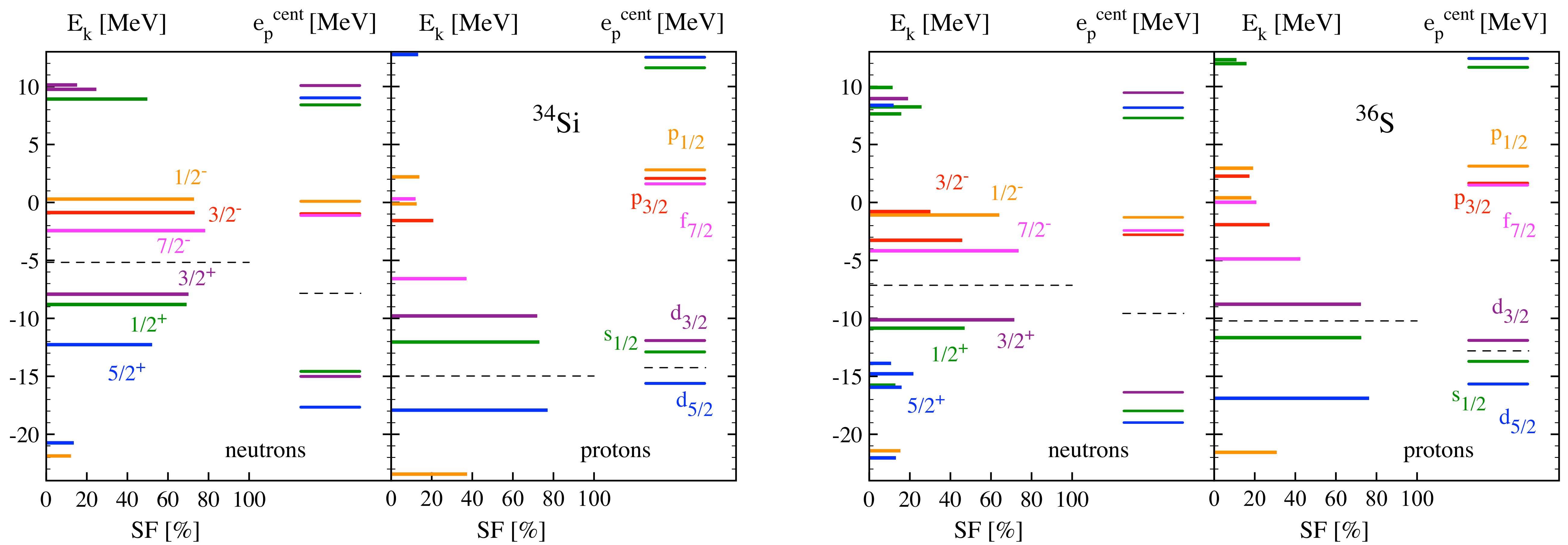
○ Largest net contribution from *s* orbitals

Spectroscopy

⦿ Green's function calculations access **one-nucleon addition & removal spectra**

One-nucleon separation energies vs. *Spectroscopic factors*

$$E_k^{\pm} \equiv \pm\left(E_k^{A\pm1} - E_0^{A}\right) \qquad SF_k^{\pm} \equiv \sum_p S_k^{\pm pp}$$

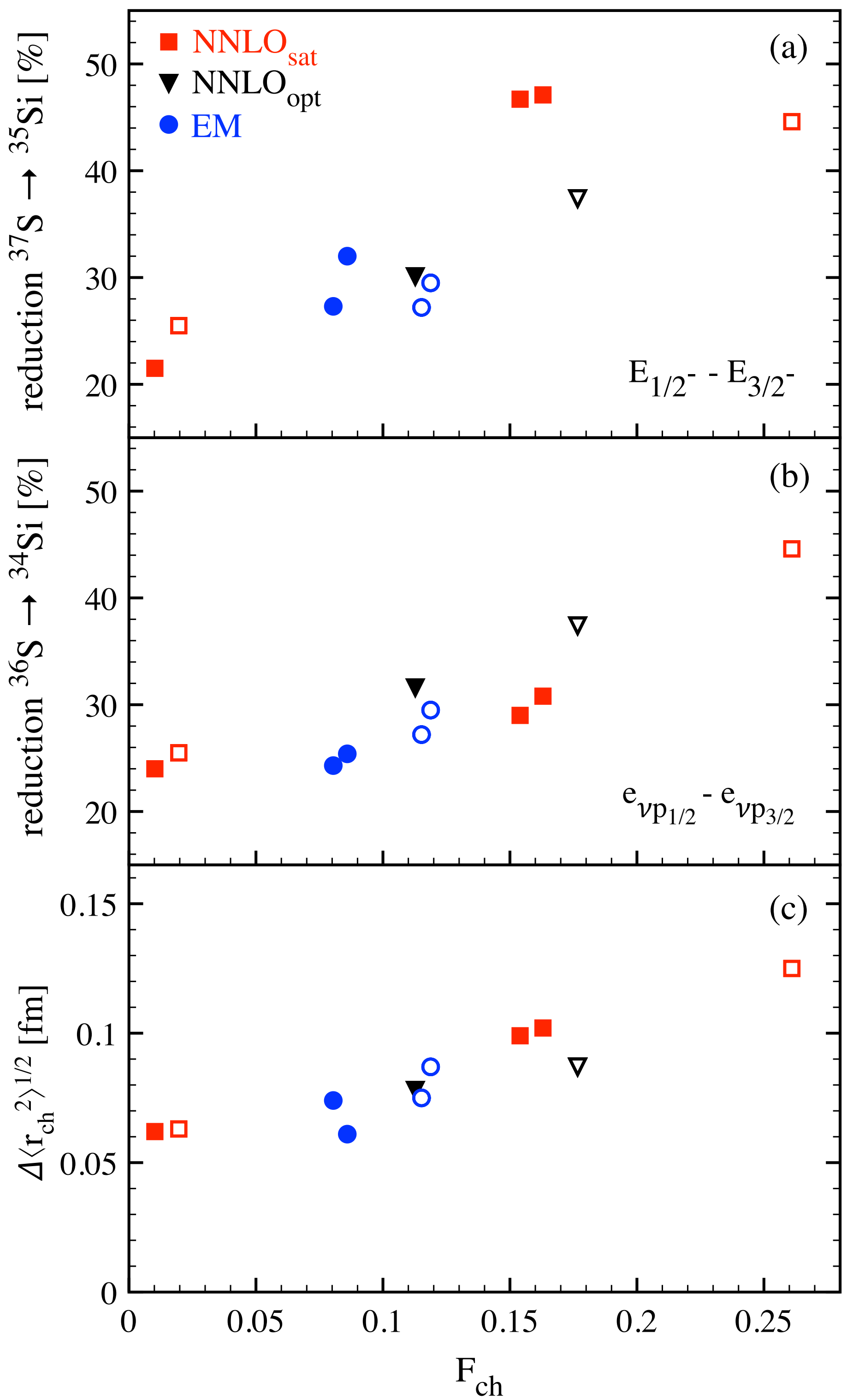


⦿ In addition, **effective single-particle energies** can be reconstructed for interpretation

$$e_p = \sum_{k\in\mathcal{H}_{A-1}} E_k^- \, S_k^{-pp} + \sum_{k\in\mathcal{H}_{A+1}} E_k^+ \, S_k^{+pp}$$

Bubble and spin-orbit

⊙ **Correlation** between bubble structure and reduction of spin-orbit splitting?



Separation energies

○ Different *H*s lead to very different depletions

○ Calculations support existence of a correlation

Effective single-particle energies

○ Lower reduction of s.o. splitting

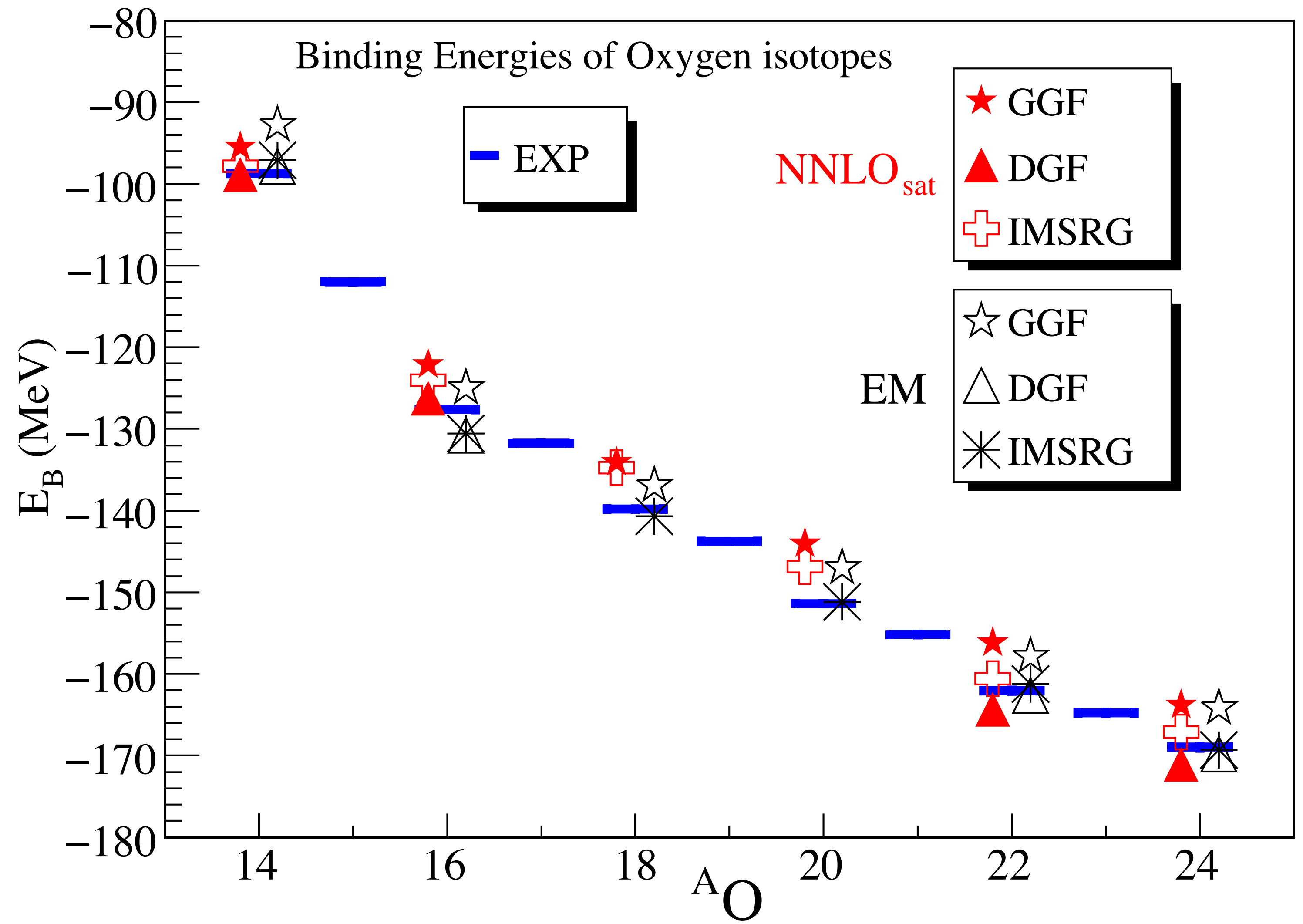
○ Linear correlation holds also for ESPEs

Charge radius difference (^{36}S-^{34}Si)

○ Radius difference also correlates with F_{ch}

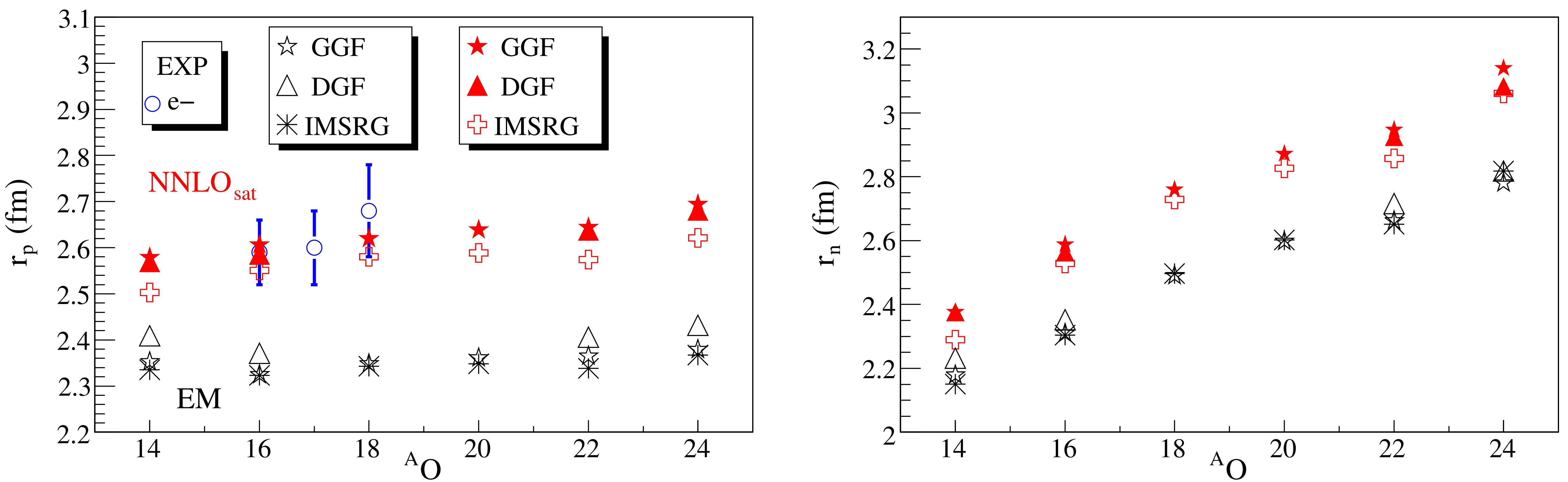
○ Motivation for measuring ^{34}Si radius

Oxygen energies



- **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)
  - How do they perform on other observables, e.g. radii?

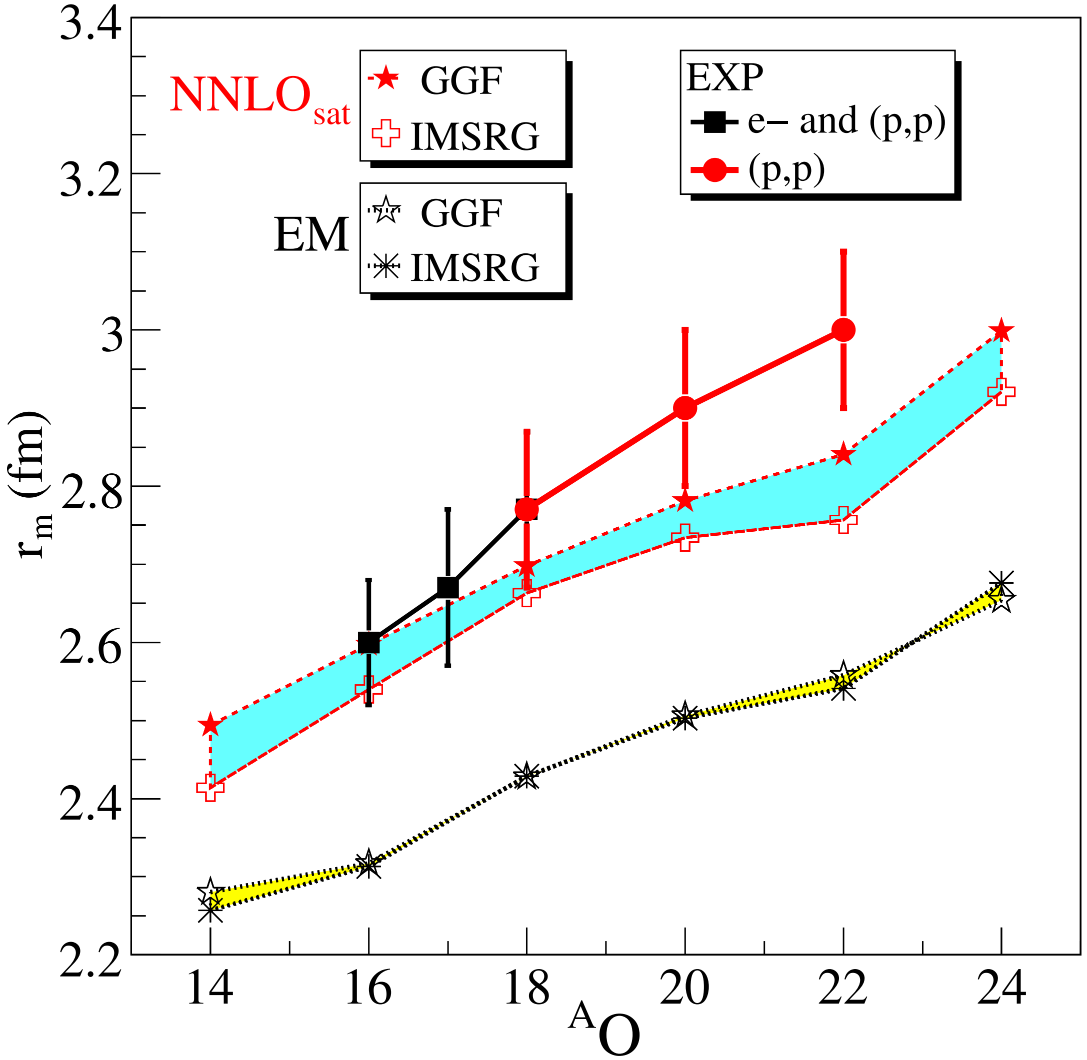
Point-proton and point-neutron radii



- **Uncertainty** from using different many-body schemes 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?**

Oxygen matter radii: exp. vs theory



- ○ NNLO$_{sat}$ **improves in absolute**
- ○ (Keep in mind that ^{16}O r_{ch} is in NNLO$_{sat}$ fit)
- ○ Somewhat **similar trend with *N***
- ○ Wider many-body band ↔ Bare vs SRG?

- ⊙ Clear improvement over standard EFT interactions, but deficiencies in isospin dependence
  - ○ This could reflect in a wrong prediction for the **symmetry energy**
- ⊙ Similar conclusions from analysis of charge radii in Ca isotopes [Garcia Ruiz *et al*. 2016]
- ⊙ NNLO$_{sat}$ strategy raises **questions about methodology and predictive power**