(Ab initio) Theoretical description of nuclear observables accessible via laser spectroscopy

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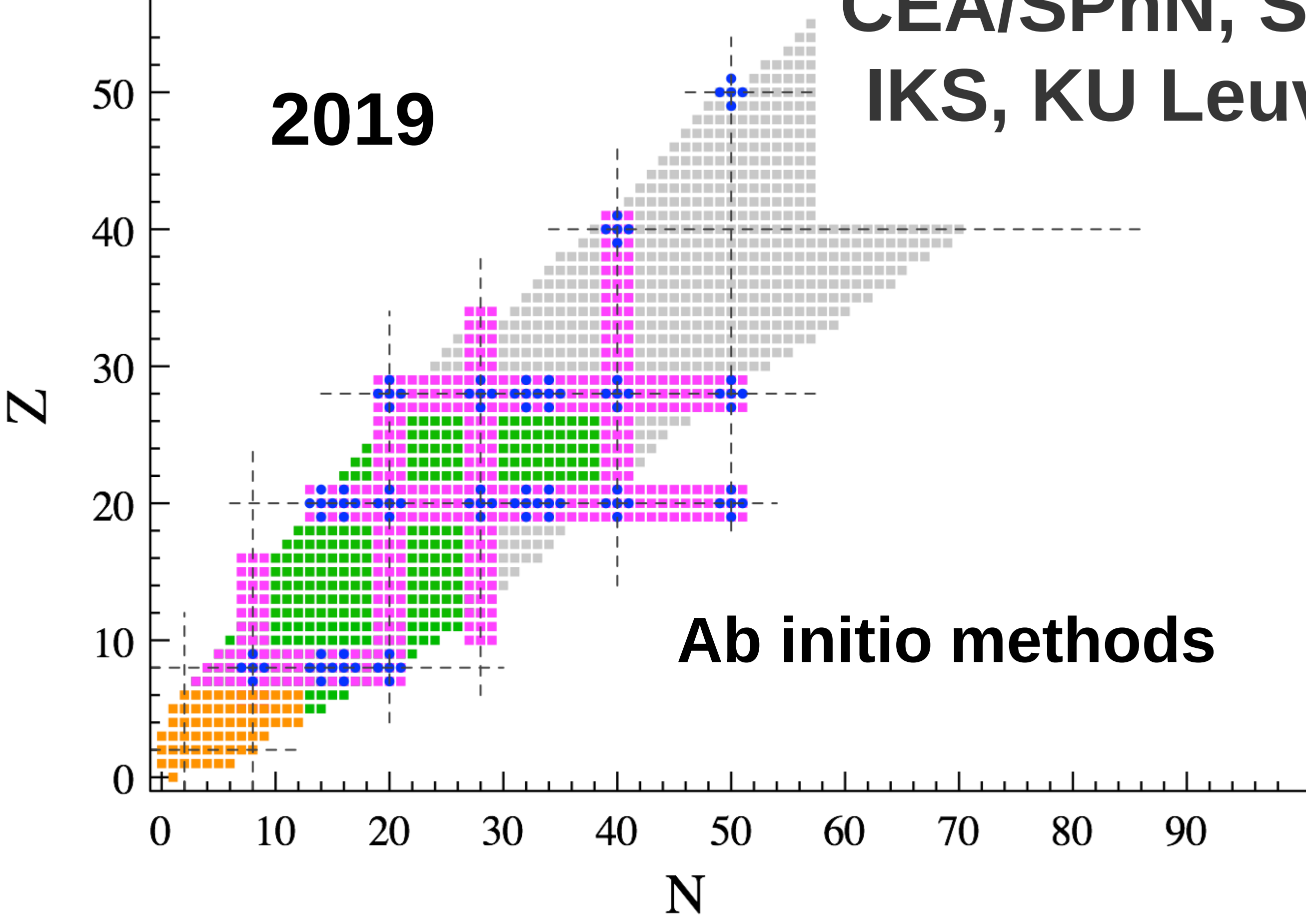

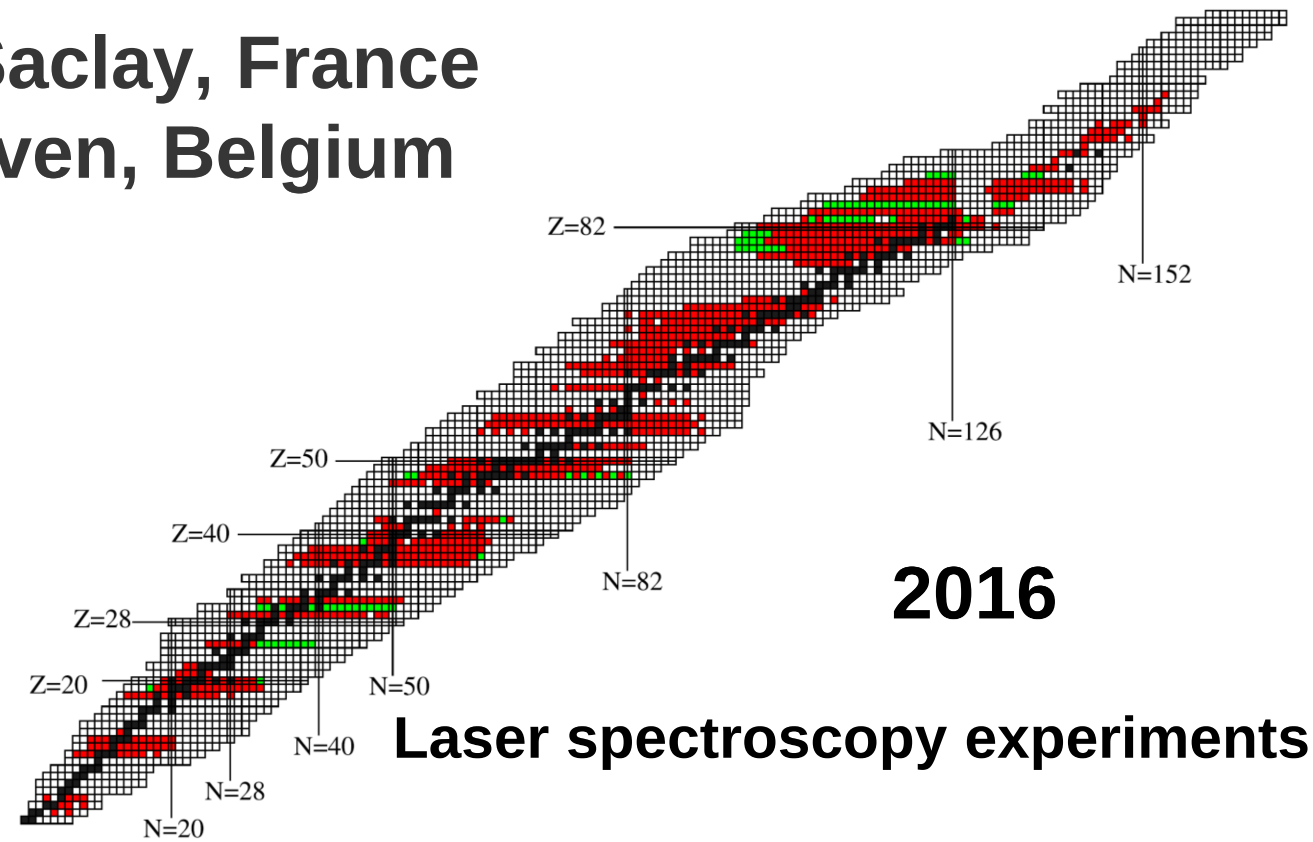

Laser spectroscopy as a tool for nuclear theories

ESNT workshop, CEA/Saclay, France, October 7th - 11th 2019

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Huge diversity of nuclear phenomena

Nucleus: bound (or resonant) state of *Z* protons and *N* neutrons

Several scales at play:

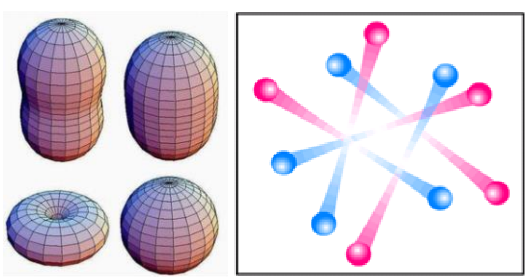
p & n momenta ~ **10^8** eV

Separation energies ~ **10^7** eV

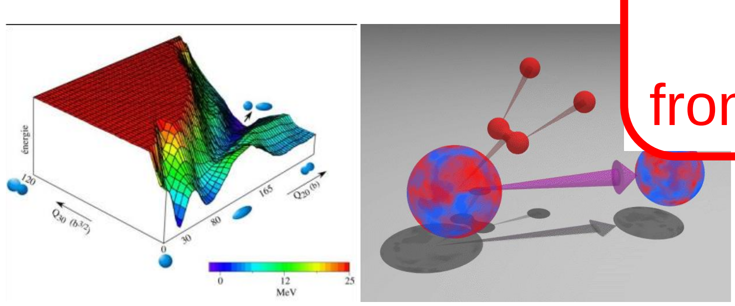
Vibrational excitations~ **10^6** eV

Rotational excitations ~ **10^4** eV

Ground state
Mass, size, superfluidity, e.m. moments…

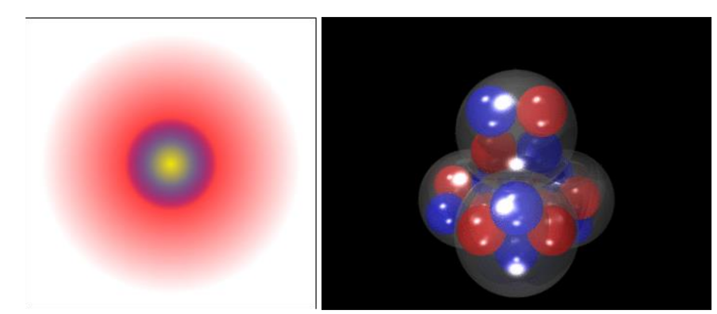


Radioactive decays
β, 2β, 0ν2β, α, p, 2p, (

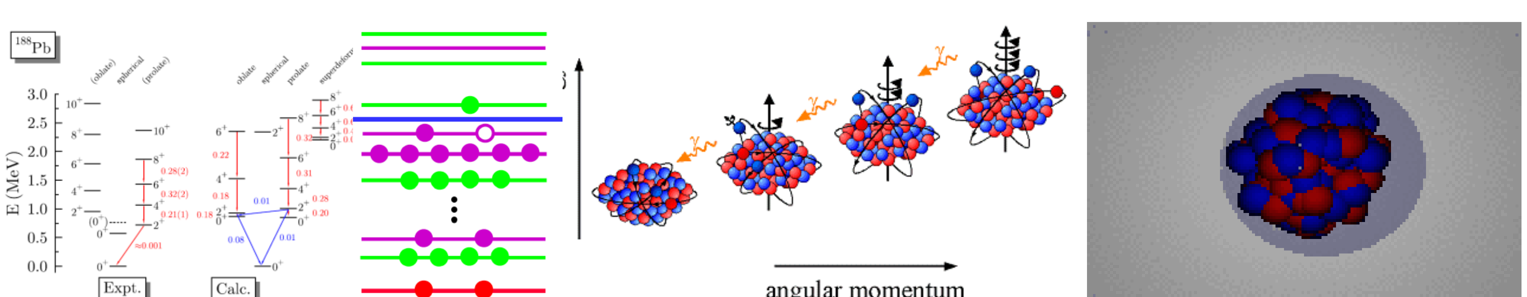


Ab initio perspective:
How does this extremely **rich phenomenology consistently emerge**
from **basic interactions** between the **nucleons**?

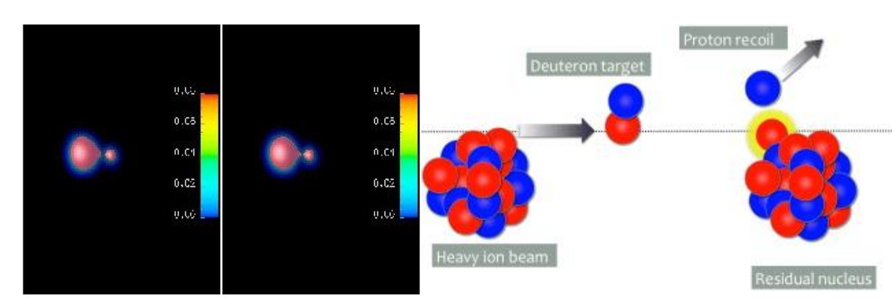
Exotic structures
Clusters, halos, …



Spectroscopy
Excitation modes



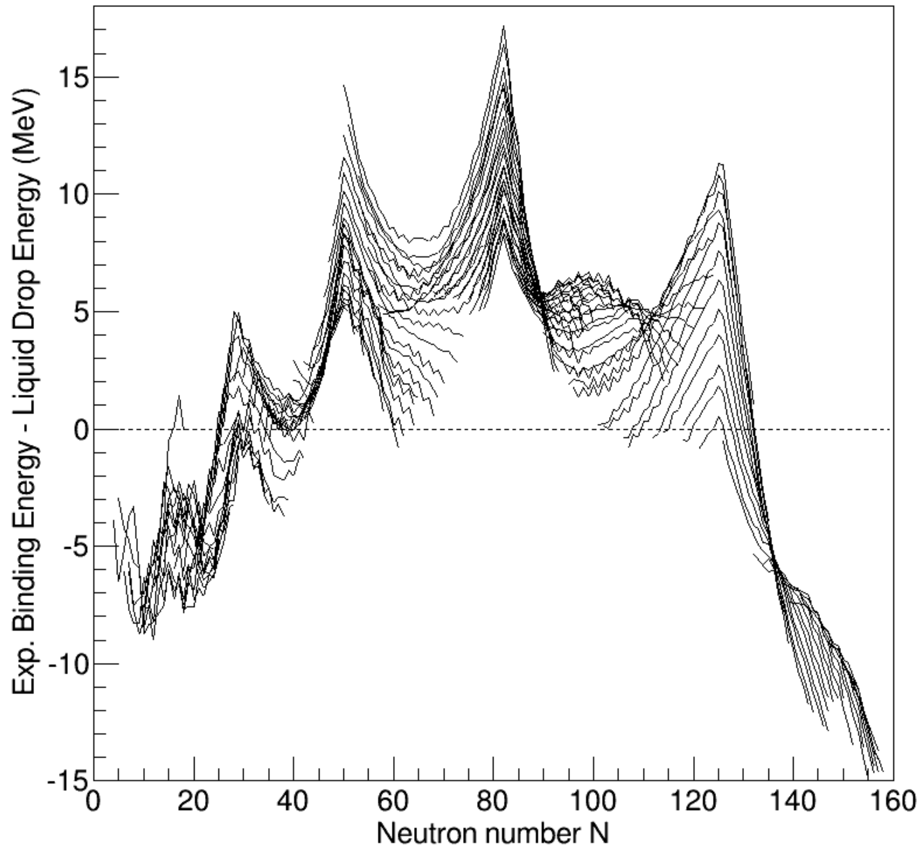
Reaction processes
Fusion, transfer, knockout, …



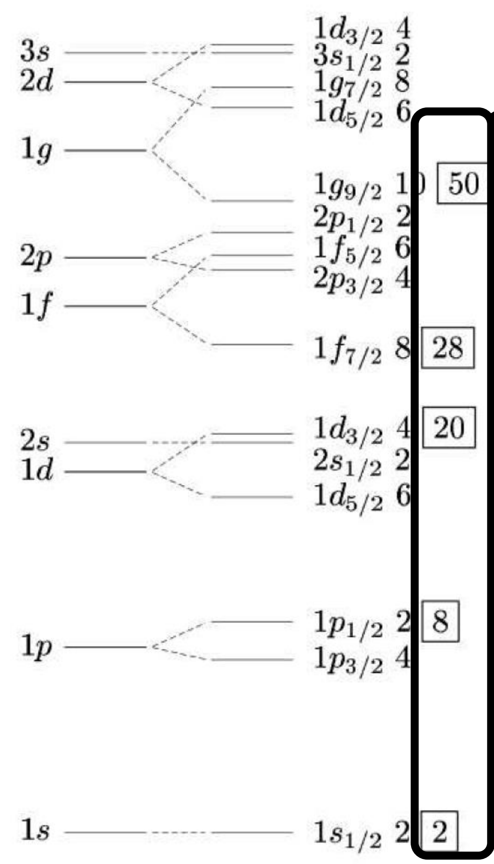
Most basic quantum nuclear structure feature: magic numbers

Measured binding energies
vs.
Liquid-drop model predictions

Over stability at N/Z = 2, 8, 20, 28, 50, 82…



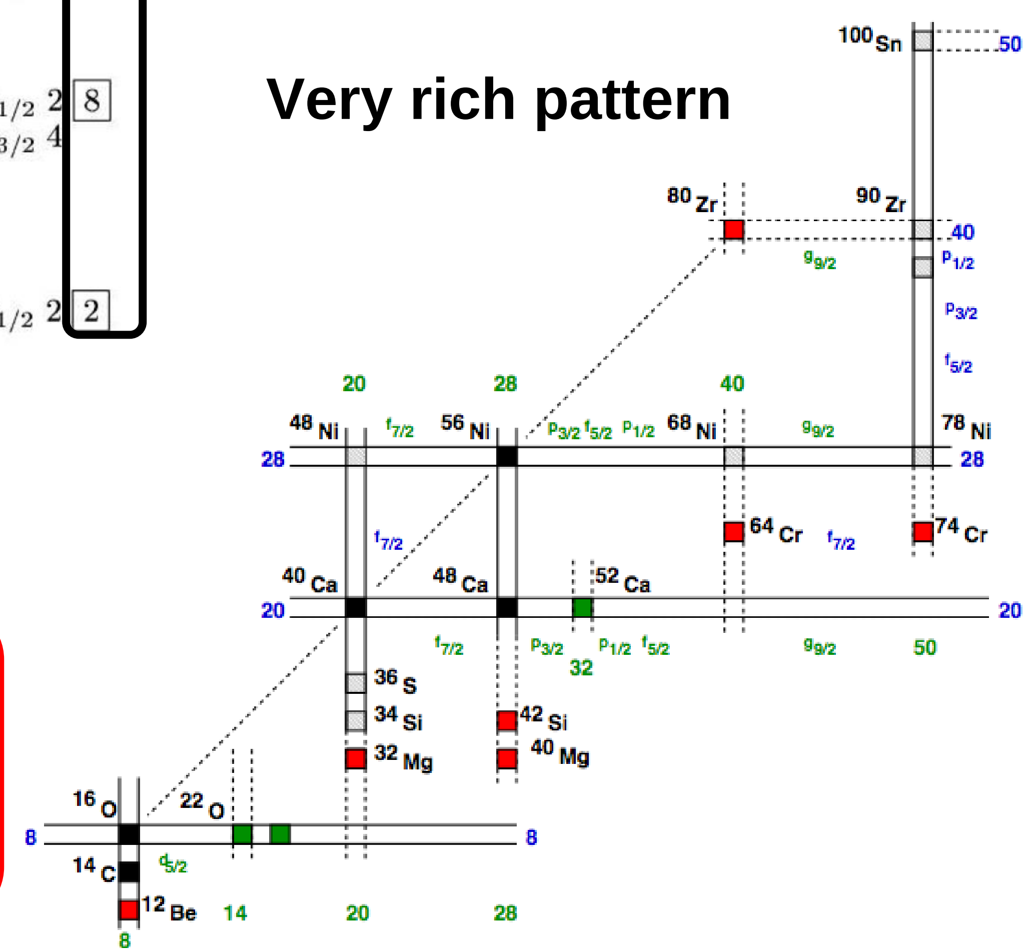
Zeroth-order model
↕
Filling of neutron/proton shells



Major closed shells
↕
Magic numbers

+
Minor closed shells
+
Modification with N-Z
+
Many-body correlations
=

Very rich pattern



→ Need to know elementary inter-nucleon interactions…

→ Need to solve the Schroedinger equation for A=2,…,82…

…not at all trivial even today!

How do they evolve across the Segrè chart?

Do they emerge from inter-nucleon interactions?

Ab initio (i.e. In medias res) quantum many-body problem

Ab initio ("from scratch") scheme = A-body Schrödinger Equation (SE)

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

A-body Hamiltonian

$$H = T + V^{2N} + V^{3N} + V^{4N} + \ldots + V^{AN}$$

A-body wave-function

5 variables x *A nucleons*

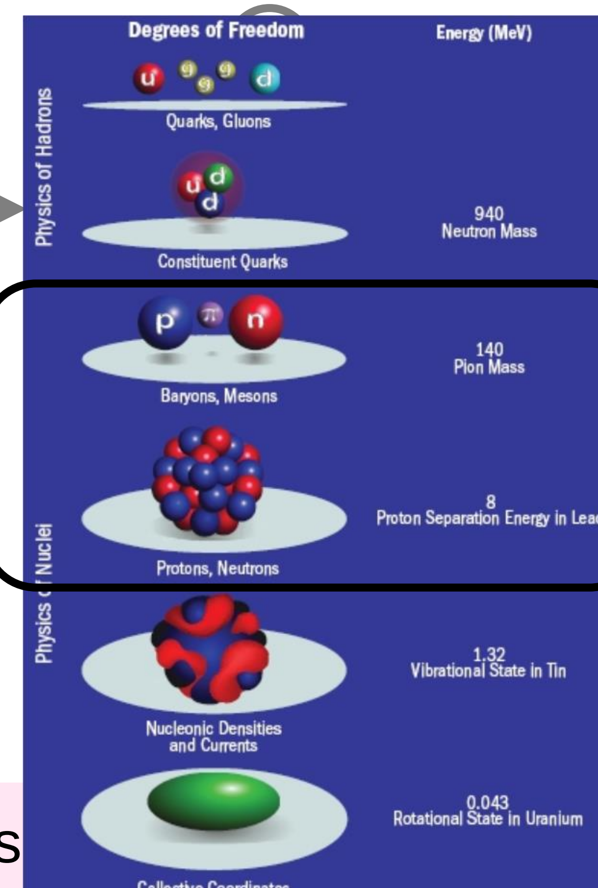
Definition

- *A* structure-less nucleons as d.o.f
- All nucleons active in complete Hilbert space
- Elementary interactions between them
- Solve A-body Schroedinger equation (SE)
- Thorough estimate of error

1 **Modeling**

1) H

2) SE



QCD 3 **Data**

?

"Ab initio"

More effective

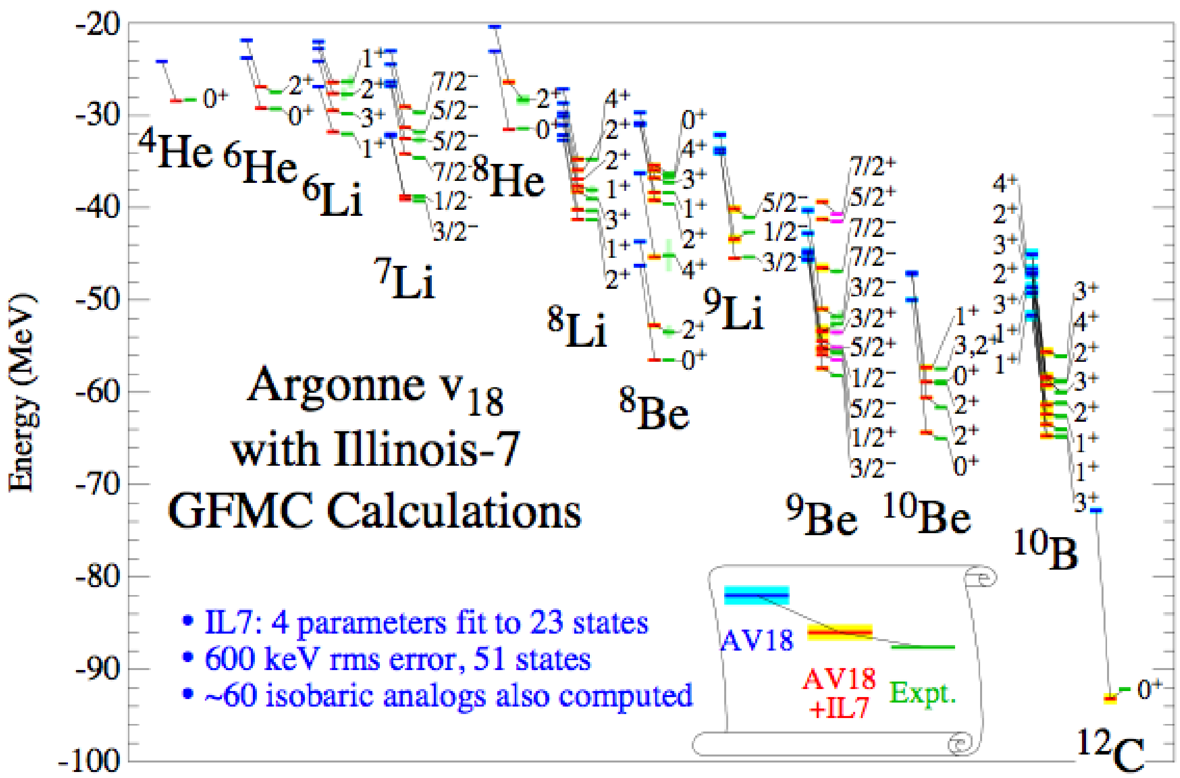
Hamiltonian&operators

Do we know the form of V^{2N}, V^{3N} etc
Do we know how to derive them from QCD?
Why would there be forces beyond pairwise?
Is there a consistent form of other operators?

Can we s... nt accuracy?
Can we do it for any A=N+Z?
Is it even reasonable to proceed this way for A≈200?
More effective approaches needed?

First ab initio calculations

- ➪ **1990's: Green function Monte Carlo approach** [Carlson, Pieper, Wiringa, Schiavilla,…]
  - ○ MC techniques to sample many-body wave function in coordinate, isospin and spin space
- ➪ **2000's: No-core shell model approach** [Vary, Barrett, Navratil, Ormand…]
  - ○ Diagonalisation of the Hamiltonian in a finite-dimensional space (but with no core!)



[Pieper & Wiringa 2001]

Nuclei simulated from "scratch"!

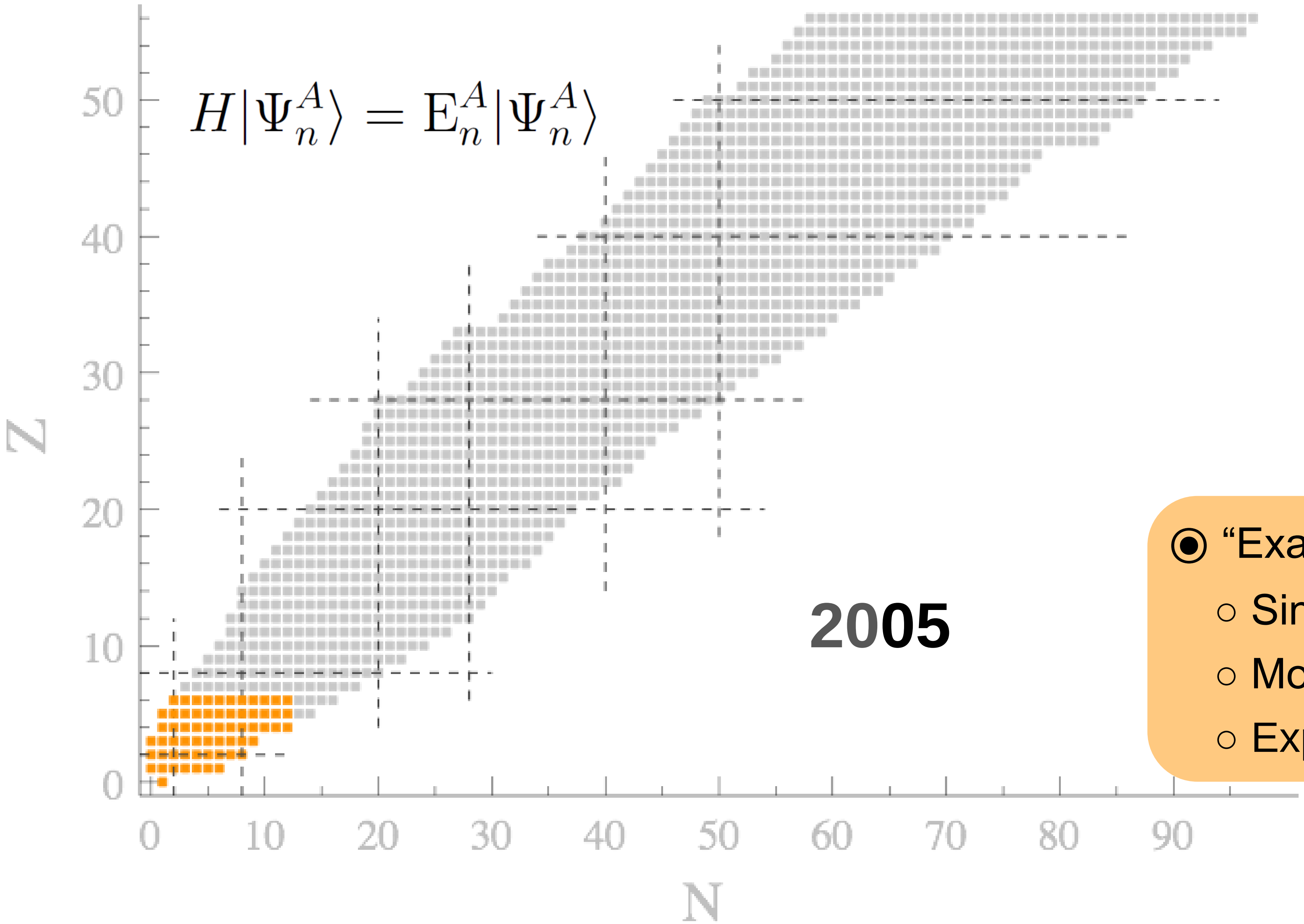
Closed the gap between elementary inter-nucleon interactions and properties of nuclei

✗ Computational effort increases exponentially/factorially with nucleon number

✗ Necessity of treating three-nucleon forces makes it more severe

→ **Approach limited to light nuclei (~A≤12)**

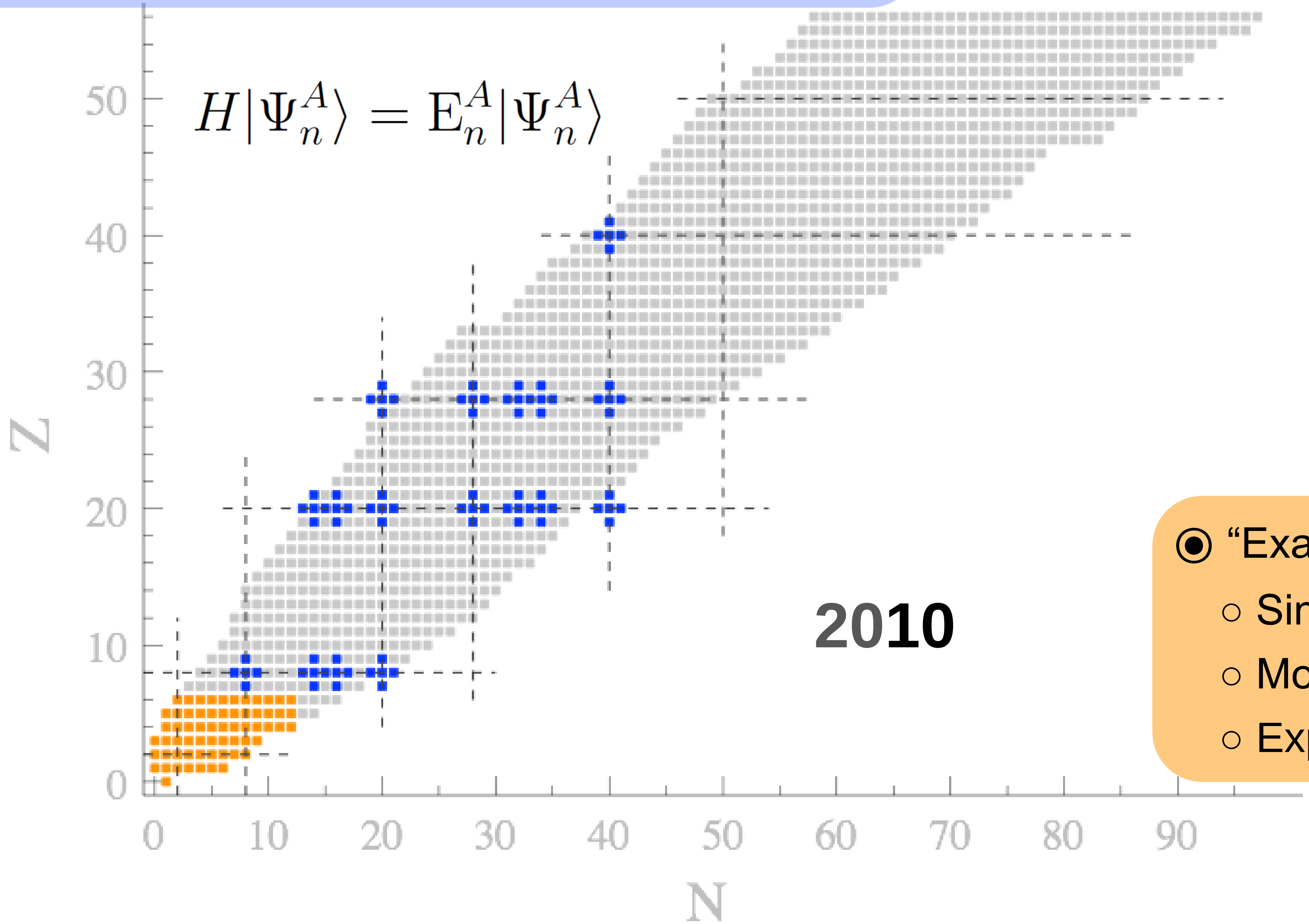
Evolution of ab initio nuclear chart



- “Exact” methods
  - Since 1980’s
  - Monte Carlo, CI, …
  - Exponential scaling

Evolution of ab initio nuclear chart

- Approximate methods for closed-shells
  - Since 2000’s
  - MBPT, DSCGF, CC, IMSRG
  - Polynomial scaling



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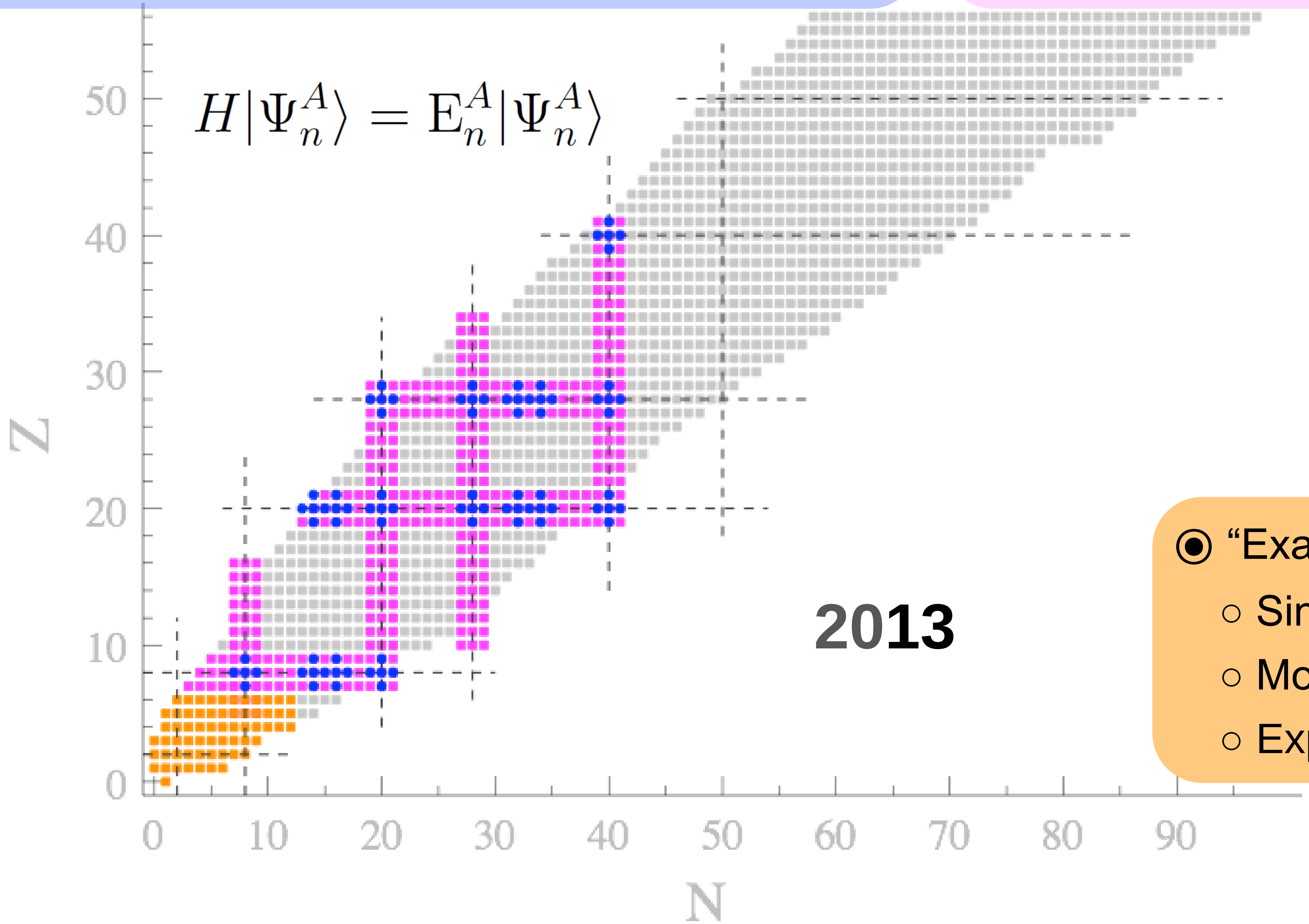
Evolution of ab initio nuclear chart

- ◉ Approximate methods for closed-shells
  - ○ Since 2000's
  - ○ MBPT, DSCGF, CC, IMSRG
  - ○ Polynomial scaling

- ◉ Approximate methods for open-shells
  - ○ Since 2010's
  - ○ BMBPT, GSCGF, BCC, MR-IMSRG, MCPT
  - ○ Polynomial scaling



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  - ○ Since 1980's
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  - ○ Exponential scaling

Evolution of ab initio nuclear chart

- Approximate methods for closed-shells
  - Since 2000's
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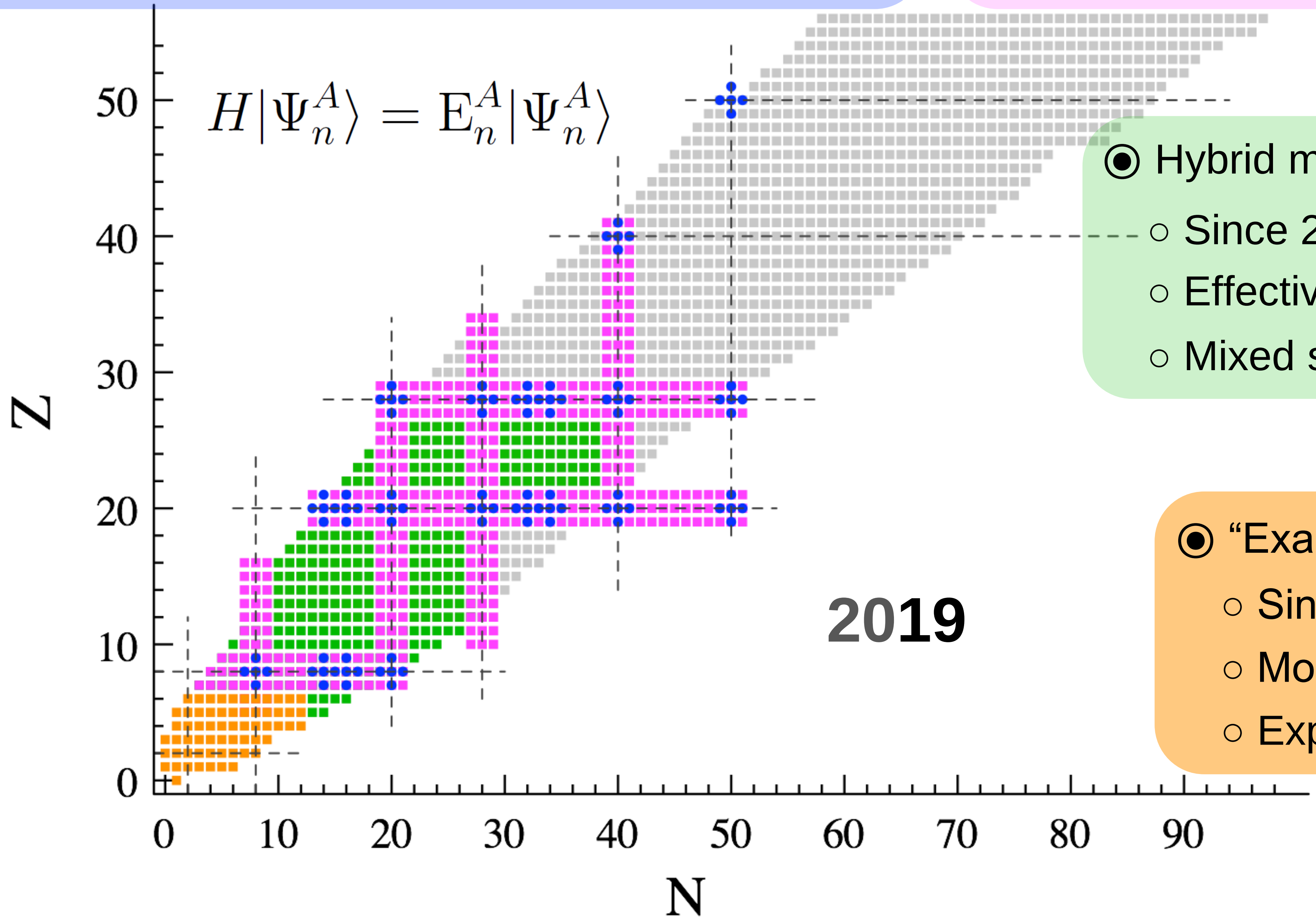


- Hybrid methods (ab initio shell model)
  - Since 2014
  - Effective interaction via CC/IMSRG
  - Mixed scaling

- "Exact" methods
  - Since 1980's
  - Monte Carlo, CI, …
  - Exponential scaling

Contents

- Introduction of the nuclear Ab initio nuclear quantum many-body problem
  - Definition and recent progress
  - Examples of recent applications
  - Some challenges and on-going developments
- Ab initio nuclear many-body problem and observables accessible via laser spectroscopy
  - Direct observables and indirect observables
  - Operators in chiral effective field theory
  - Applications in s and p shell nuclei
  - Applications in sd-pf shell nuclei
- Conclusions

Chiral EFT hamiltonians

◉ N3LO (~2010)

[Entem & Machleidt 2003, Navrátil 2007, Roth et al. 2012]

SRG λ=2.0 fm^{-1}

- First generation of ChEFT interactions (N^{3}LO 2N + N^{2}LO *3N*)
- Follows traditional ab initio strategy (fit *X*-body sector on *X*-body data)
- **Successful in light nuclei, but strong overbinding and too small radii for heavier systems**

◉ NNLO$_{sat}$ (2015)

[Ekström *et al.* 2015]

- Development prompted by inability to reproduce radii beyond light nuclei
- Data from not-so-light nuclei (*A*=14-25) included in fit + Non-local 3NF regulator
- **Good BE and radii in mid-mass but two- and few-few-body systems slightly deteriorated**

◉ N3LO$_{lnl}$ (2018)

[Entem & Machleidt 2003, Navrátil 2018]

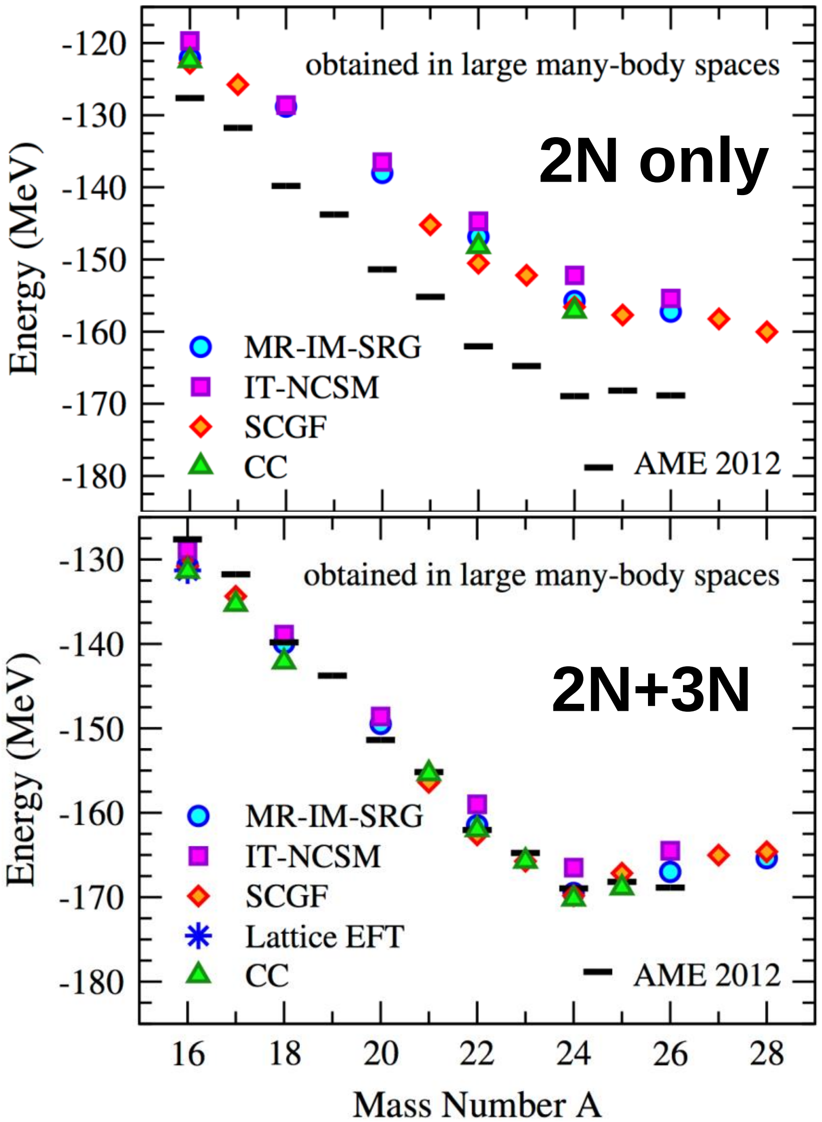
SRG λ=2.0 fm^{-1}

- Back to standard ab initio strategy but with implementation of non-local regulators
- Correct description of two- and few-body systems
- **BE and radii of mid-mass systems much improved compared to N3LO**

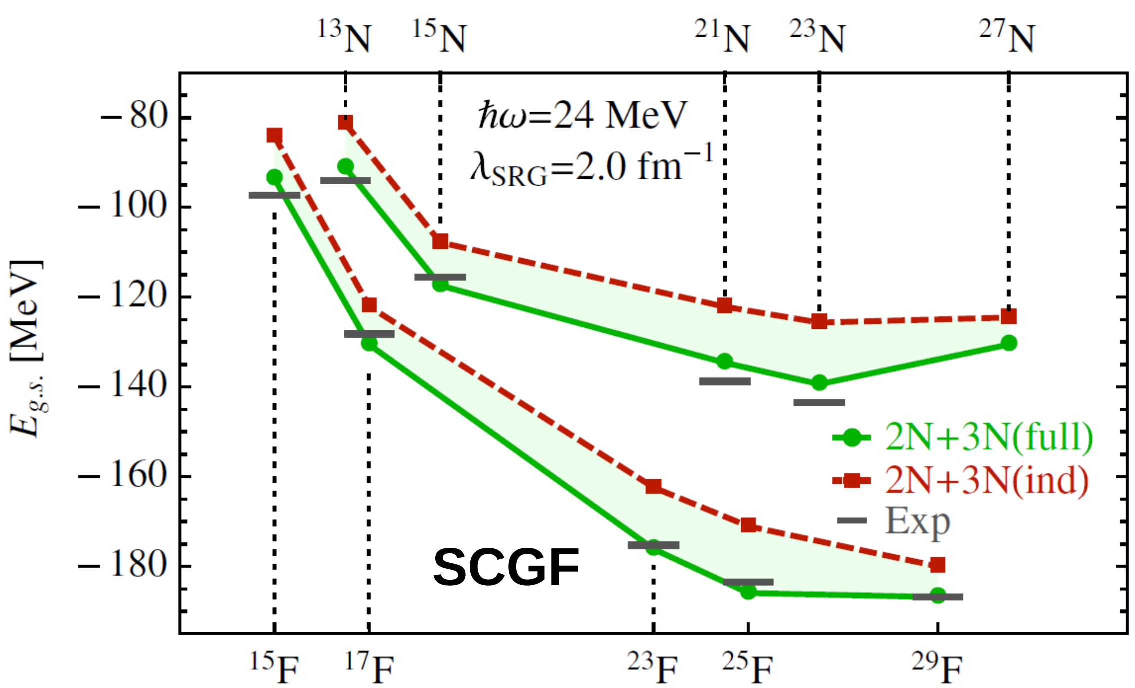
Oxygen binding energies

◉ Oxygen chain: importance of **three-body forces** and **benchmark** case for ab initio calculations

◉ N3LO (~2010)



[Hebeler et al. 2015]



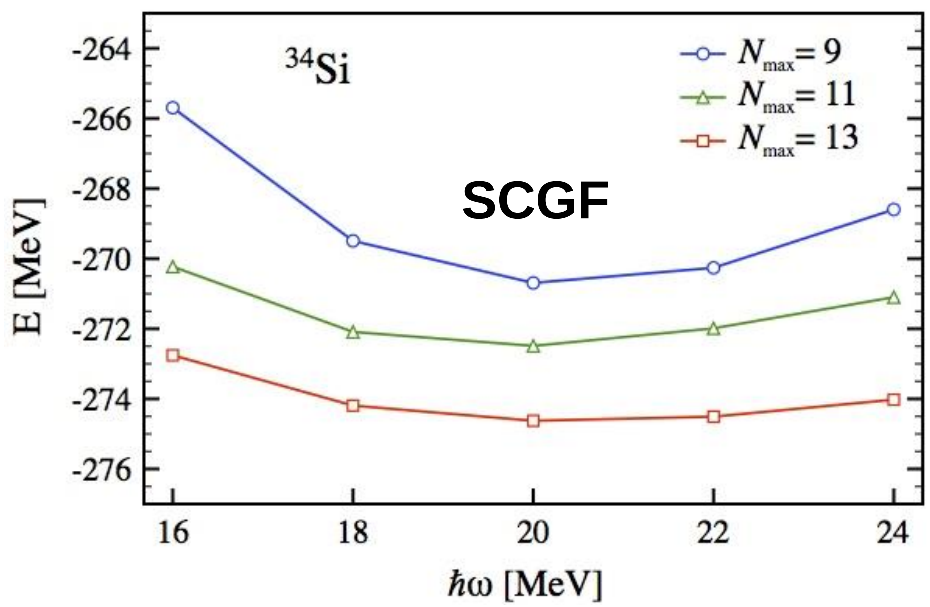
[Cipollone, Barbieri & Navrátil 2013]

✓ Neighbouring F & N chains
✓ Results are nicely consistent
✓ Interactions seem to work very satisfactorily

✓ Different methods yield consistent results
✓ 3N interaction mandatory
✓ Correct trend and drip-line location at N=16

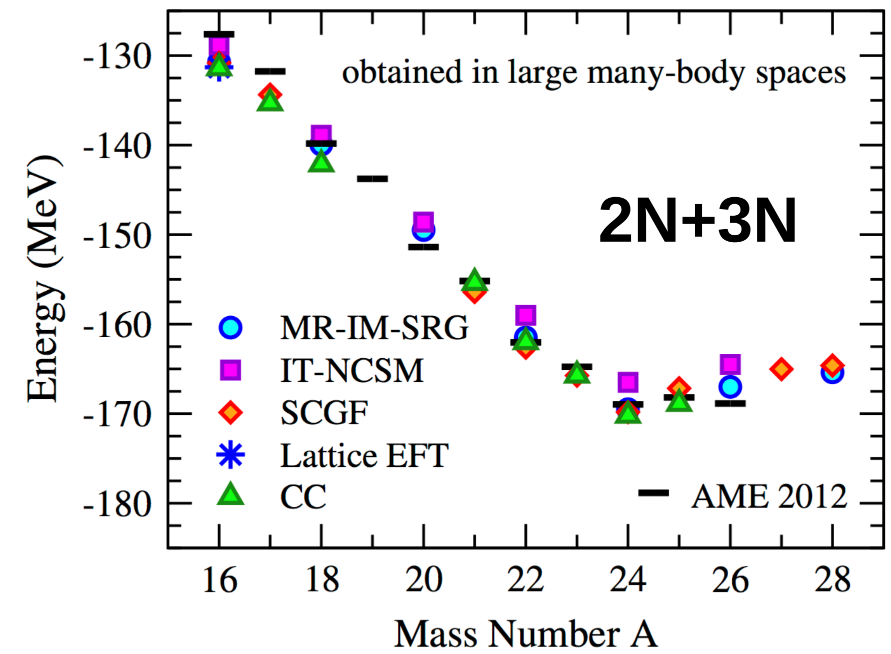
Sources of uncertainty

◉ **Model space** truncation typically up to 1%



[Duguet et al. 2016]

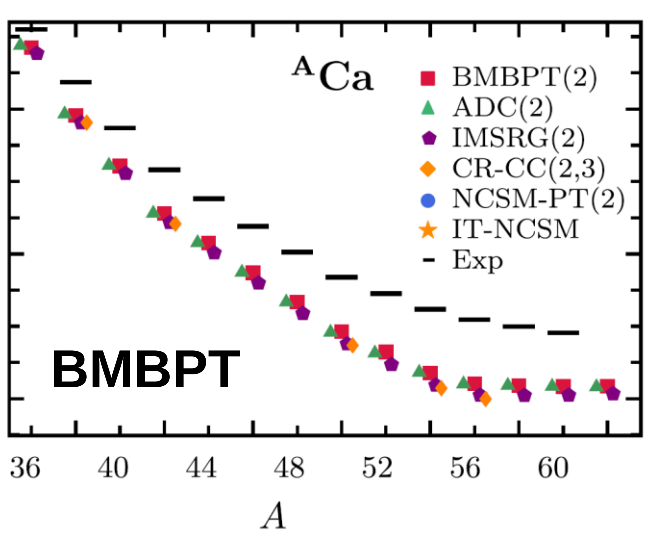
◉ **Many-body truncation** typically 2-3%



[Hebeler et al. 2015]

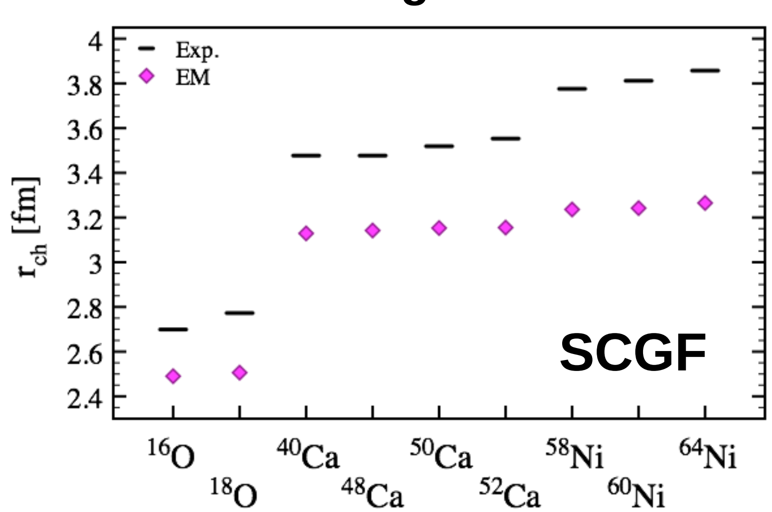
◉ **Difference with data up to 10-15% in Ca-Ni region with N3LO**

Energy

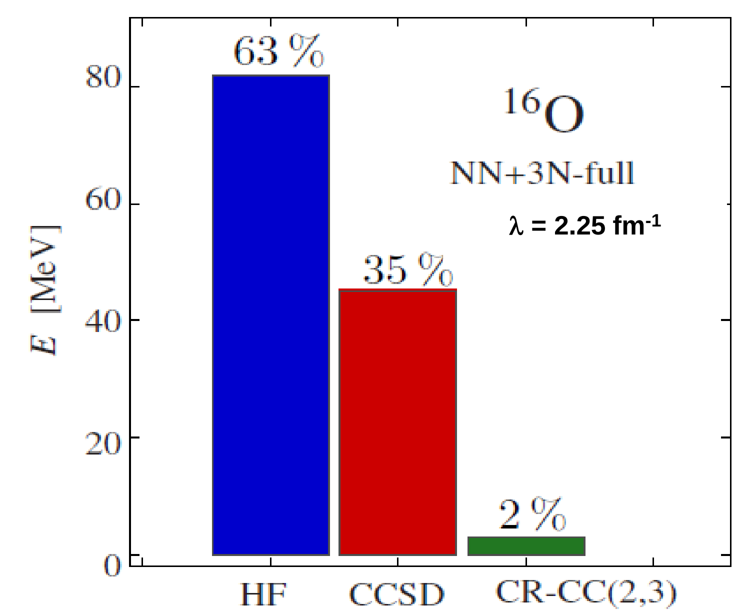


[Tichai et al. 2018]

Charge radius



[Somà, et al. 2019]



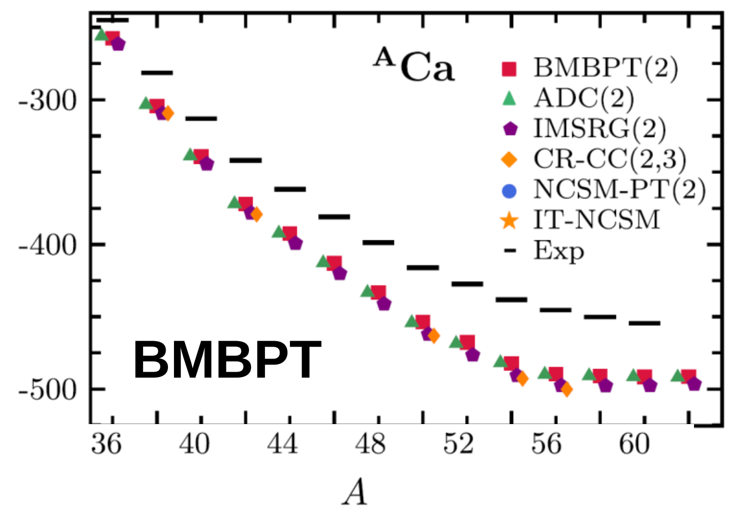
[Binder et al. 2015]

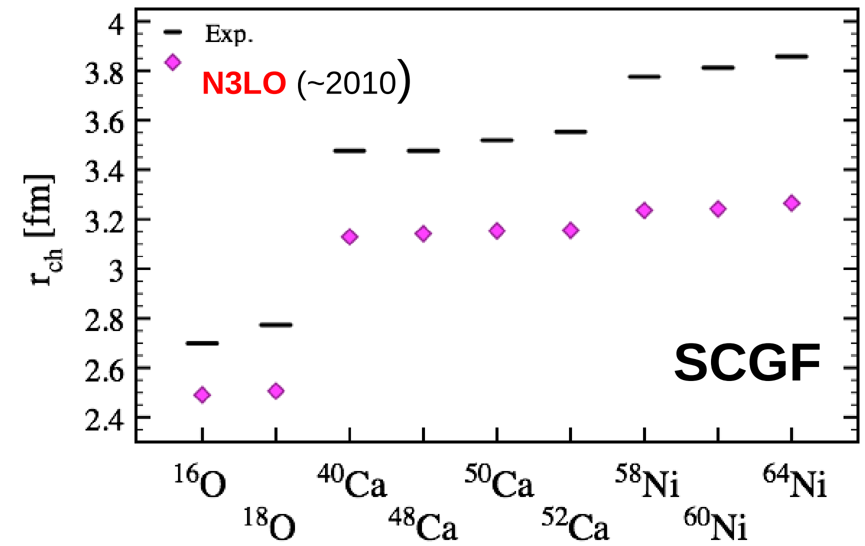
Largest uncertainty from input Hamiltonian

→ Improved Hamiltonians needed

Charge radii in medium-mass nuclei

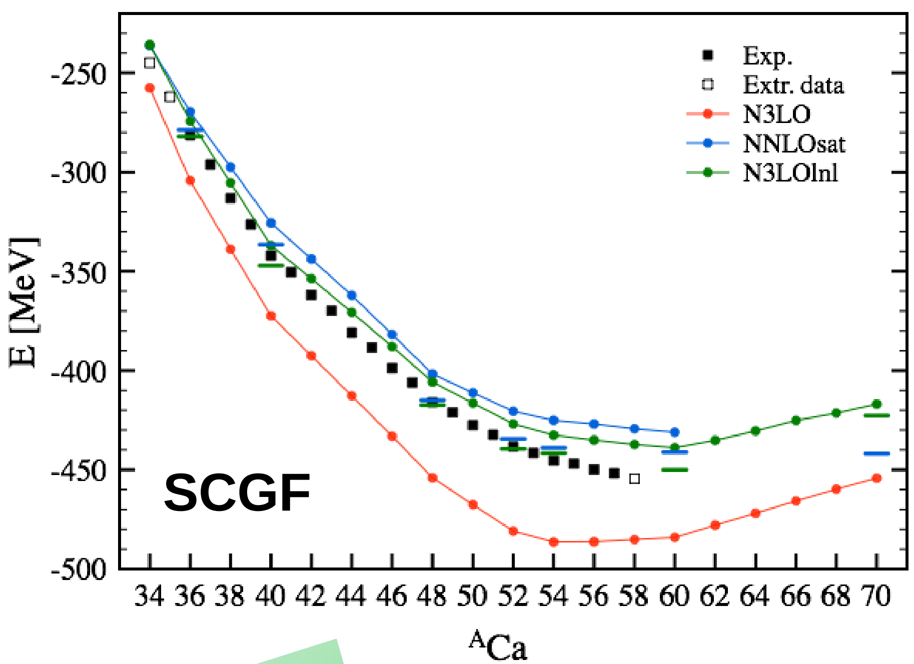
◉ **N3LO** (~2010)

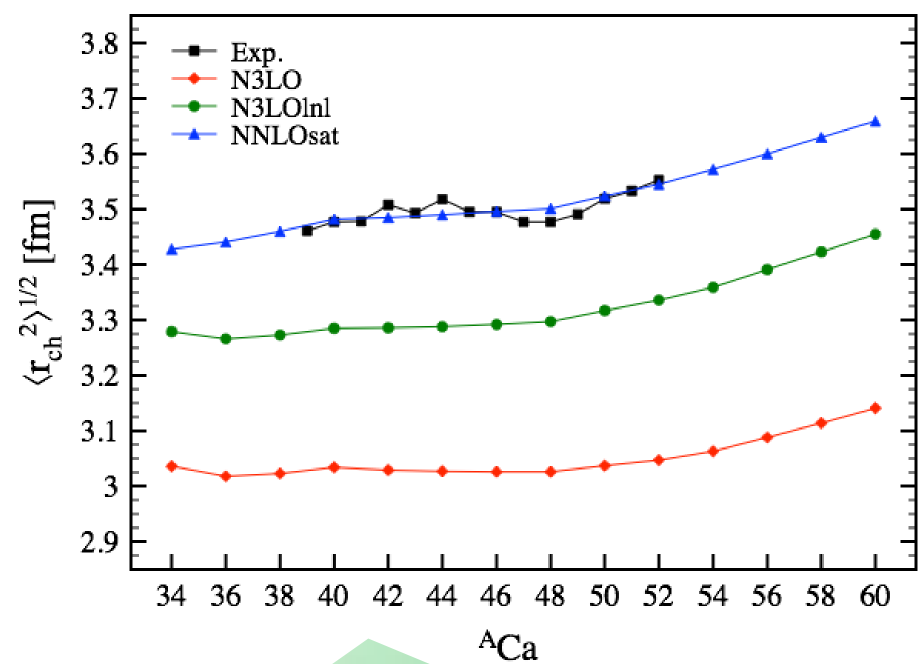




[Somà *et al.* 2019]

◉ Newly developed Hamiltonians improves the situation





[Somà *et al.* 2019]

○ New interactions correct for overbinding

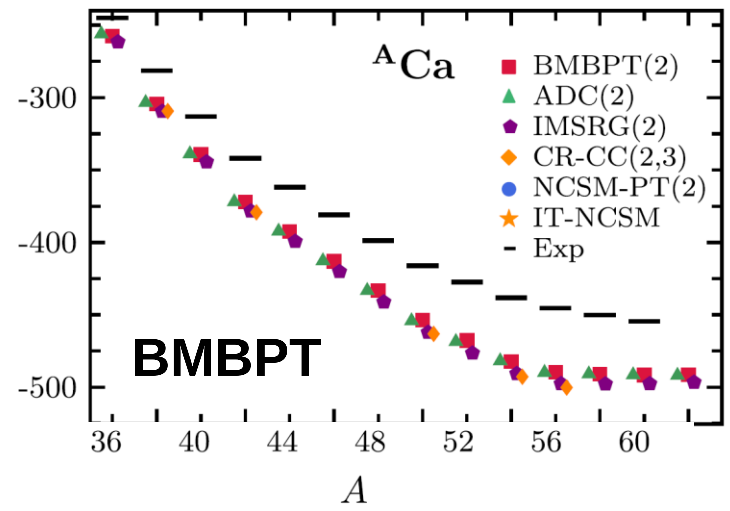
○ Full correlations needed

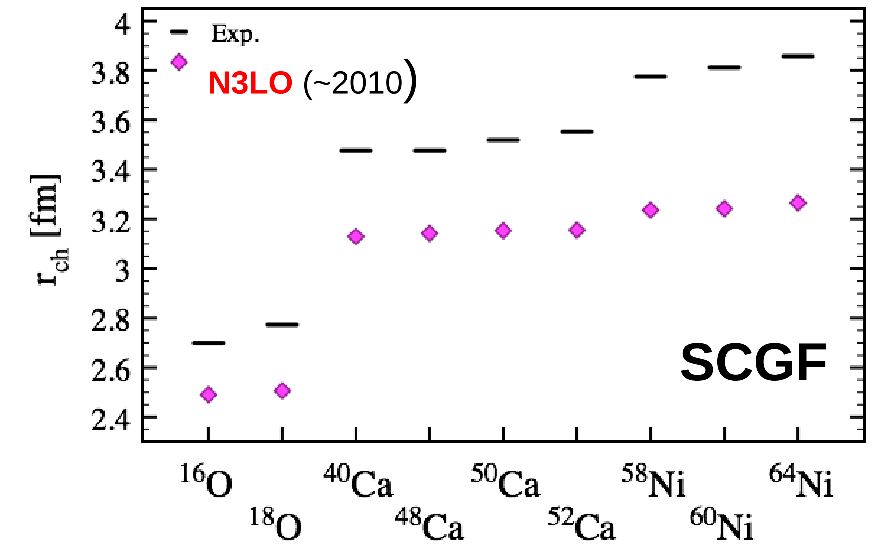
○ Radii OK when fitted!

○ Considerable improvement N3LO → N3LO$_{lnl}$

Charge radii in medium-mass nuclei

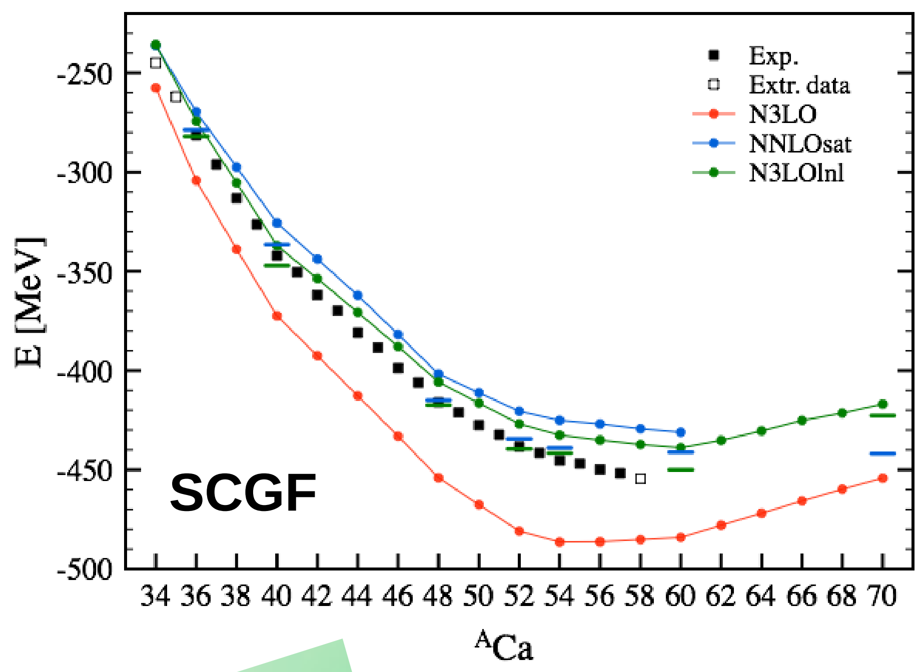
◉ **N3LO** (~2010)



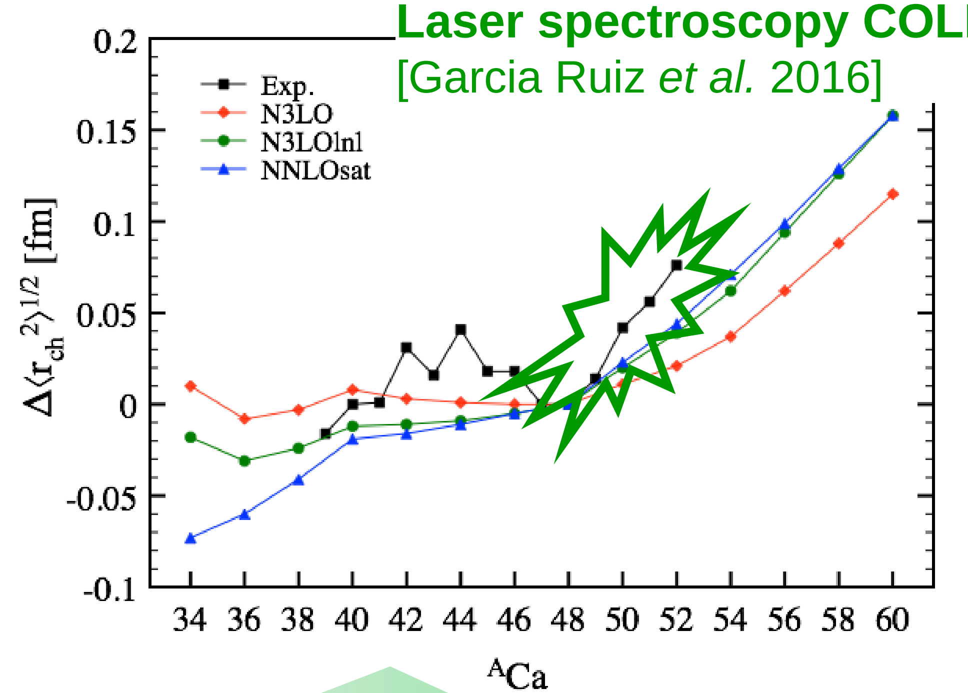


[Somà *et al.* 2019]

◉ Newly developed Hamiltonians improves the situation



Laser spectroscopy COLLAPS @ ISOLDE
[Garcia Ruiz *et al.* 2016]



[Somà *et al.* 2019]

○ New interactions correct for overbinding

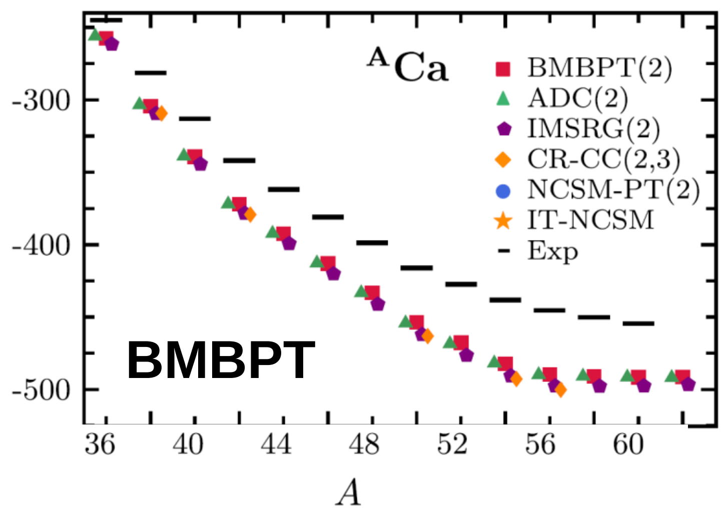
○ Full correlations needed

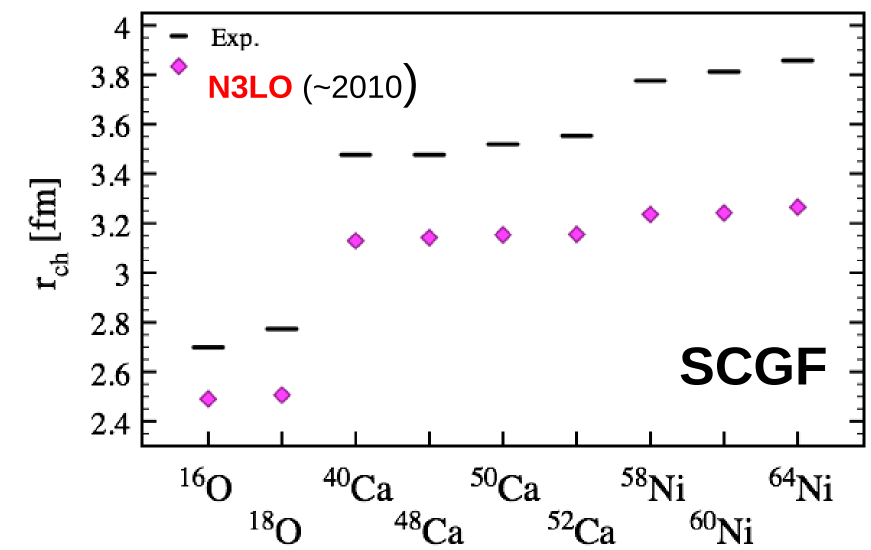
○ N3LO$_{lnl}$ follows NNLO$_{sat}$ except for proton-rich systems

○ $^{40\text{-}48}$Ca trend : requires np-nh excitations of higher ranks

Charge radii in medium-mass nuclei

◉ **N3LO** (~2010)

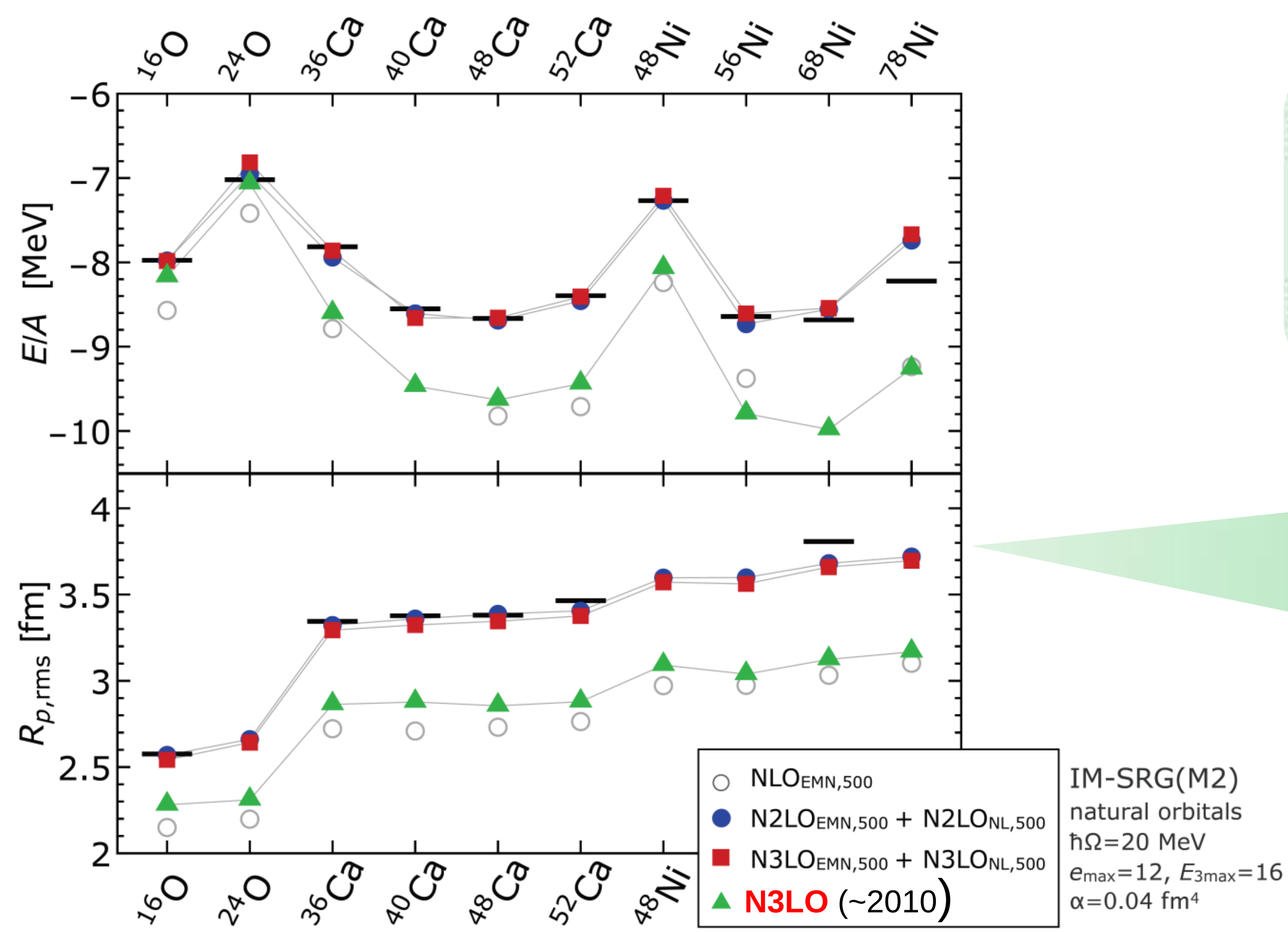




[Somà *et al.* 2019]

◉ Even more recent generation seems to get it all…

[Huther *et al.* 2019, unpublished]



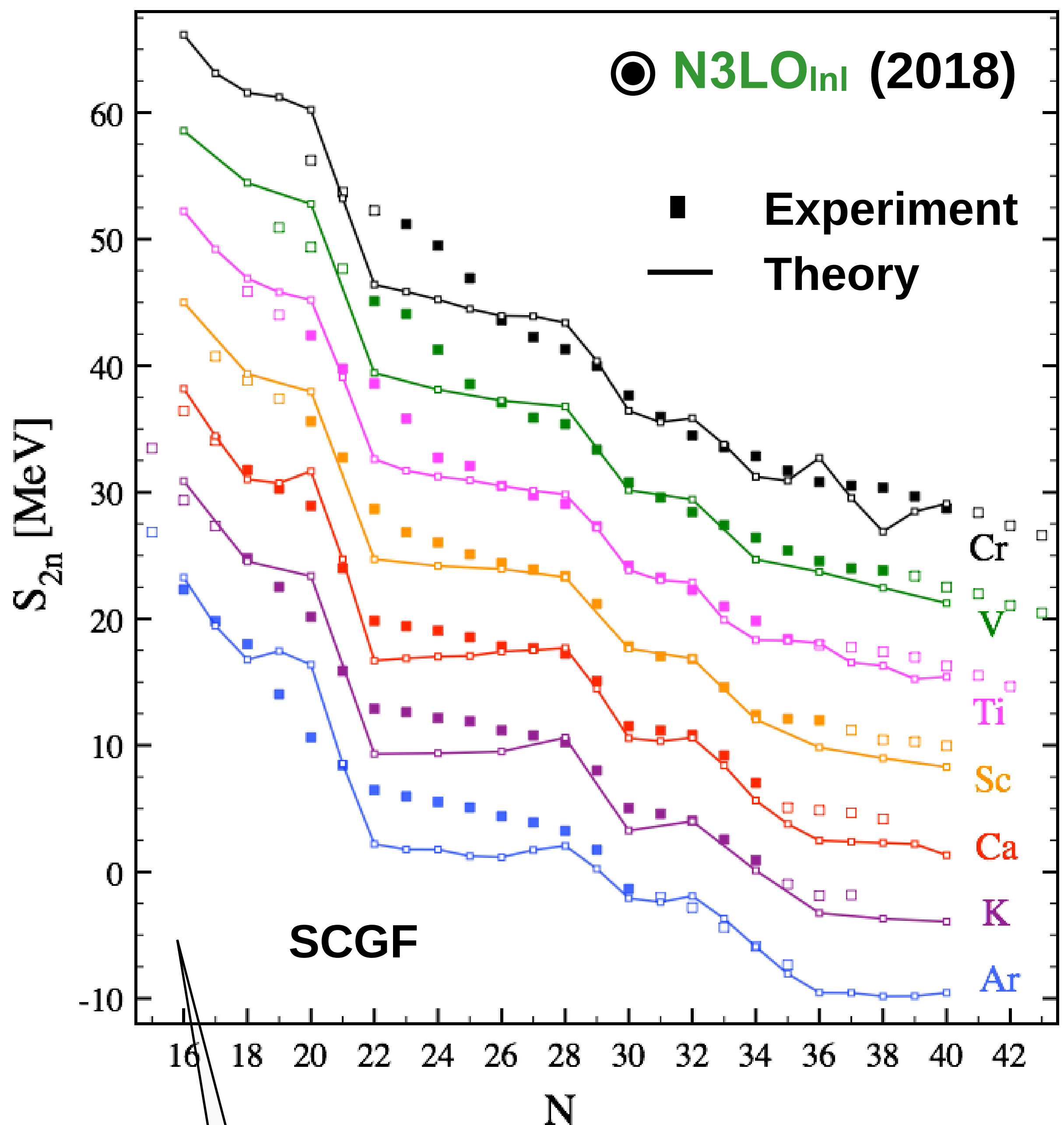
- ○ Consistent family at NLO, N^{2}LO, N^{3}LO
- ○ Non-local 3N regulator
- ○ C_D LEC tuned to BE(^{16}O) (^{4}He slightly relaxed)

- ○ Excellent reproduction of ground-state energies
- ○ Excellent agreement for radii
- ○ Net improvement from NLO to N^{2}LO
- ○ Stable from N^{2}LO to N^{3}LO

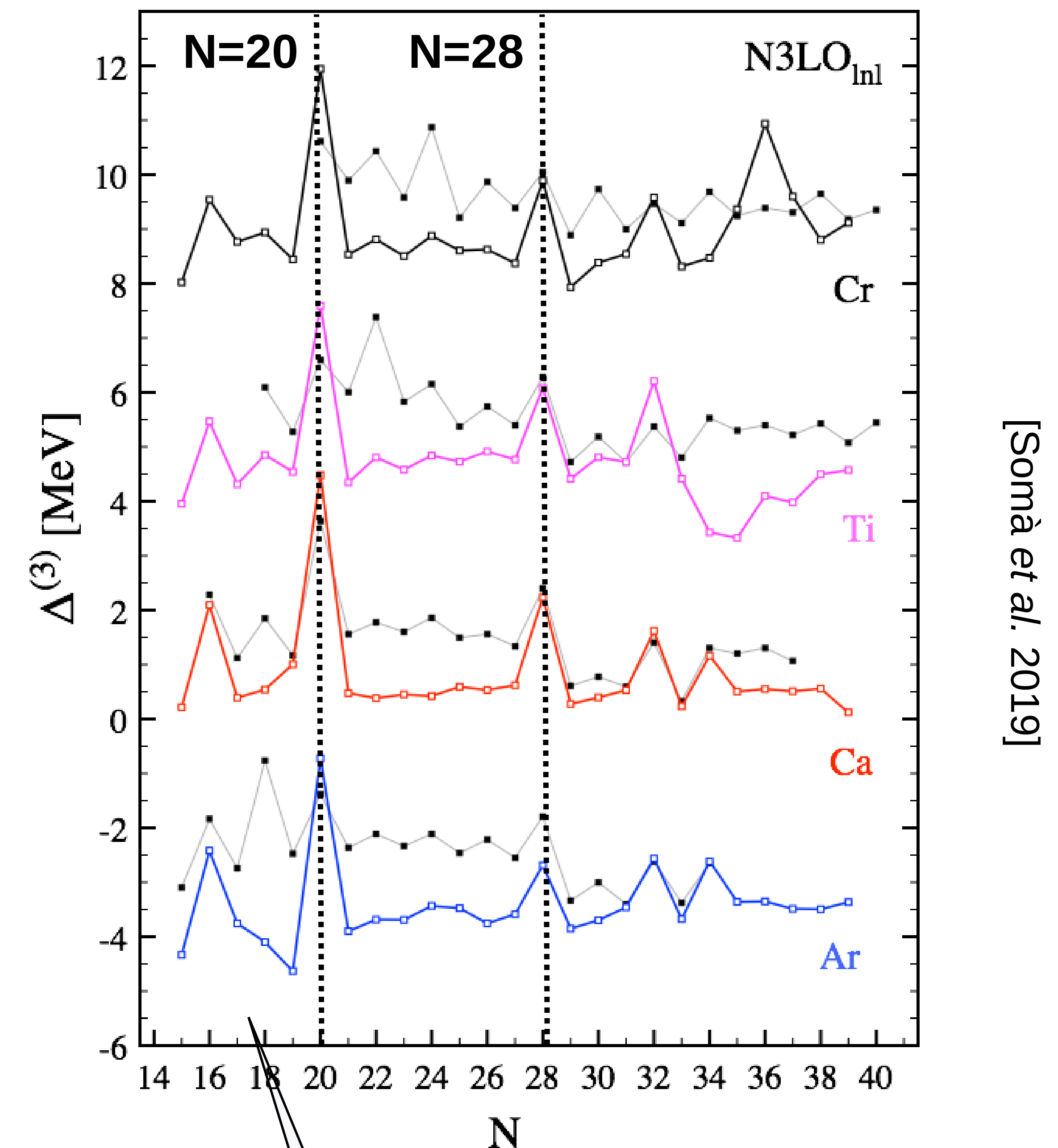
◉ Charge radii provide stringent tests of nuclear interactions via ab initio calculations of mid-mass chains

Ab initio emergence of N=20 and N=28 magic numbers

Two-neutron separation energy



Gap size



✗ *N* = 20 emerges but overestimated

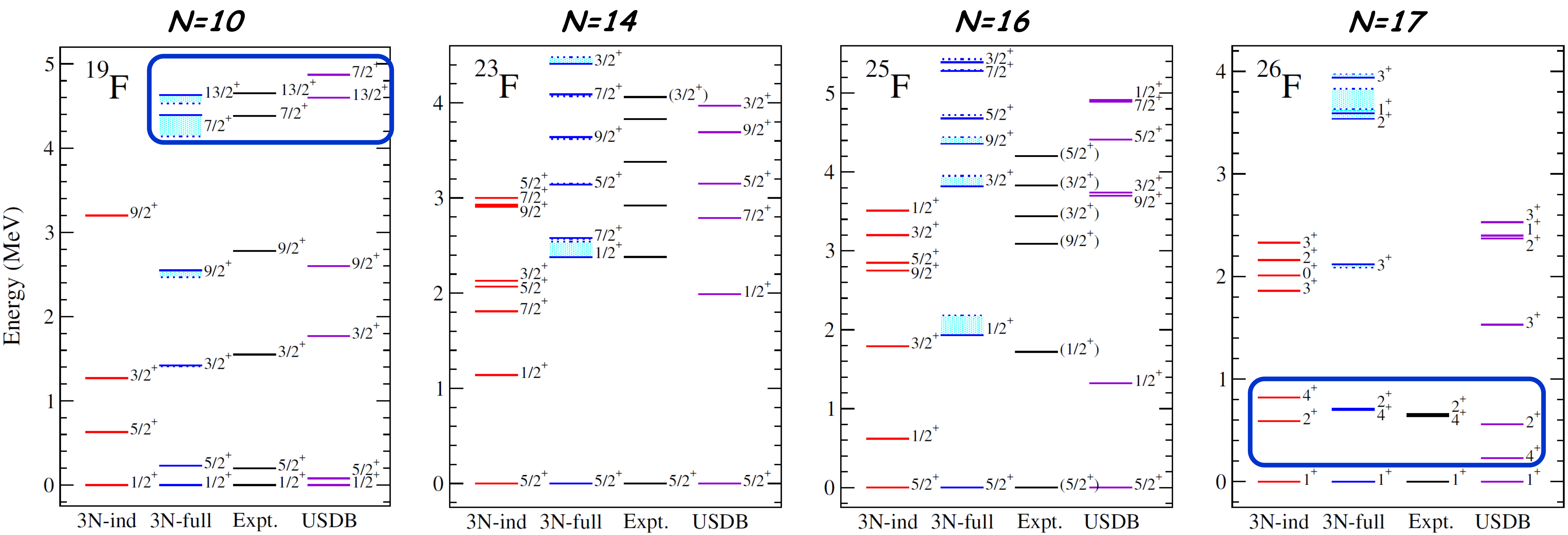
✓ Good agreement for *N* ≥ 28

✓ Main gaps nicely emerge!

✗ Pairing too weak in $f_{7/2}$

Spectra of Fluorine isotopes

- Excitation spectra of (neutron-rich) ^{19,23,25,26}F from *ab initio* sd shell model
  - **N3LO (~2010)**
    - ○ Hybrid method = ab initio shell model (core ^{16}O and valence space H from IMSRG)



✓ Very satisfactory account of experimental data

✓ 3N interaction mandatory for correct density of states and ordering

✓ As good as best sd shell empirical USDB interaction (i.e. traditional shell model)

[Stroberg *et al.* 2016]

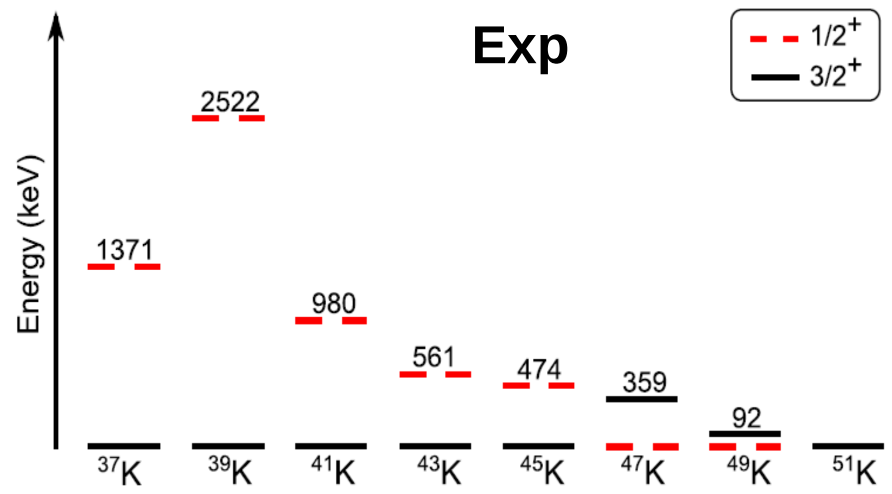
→ Confrontation with spectroscopic data in sd nuclei can now be based on ab initio scheme!

Spectra of K isotopes

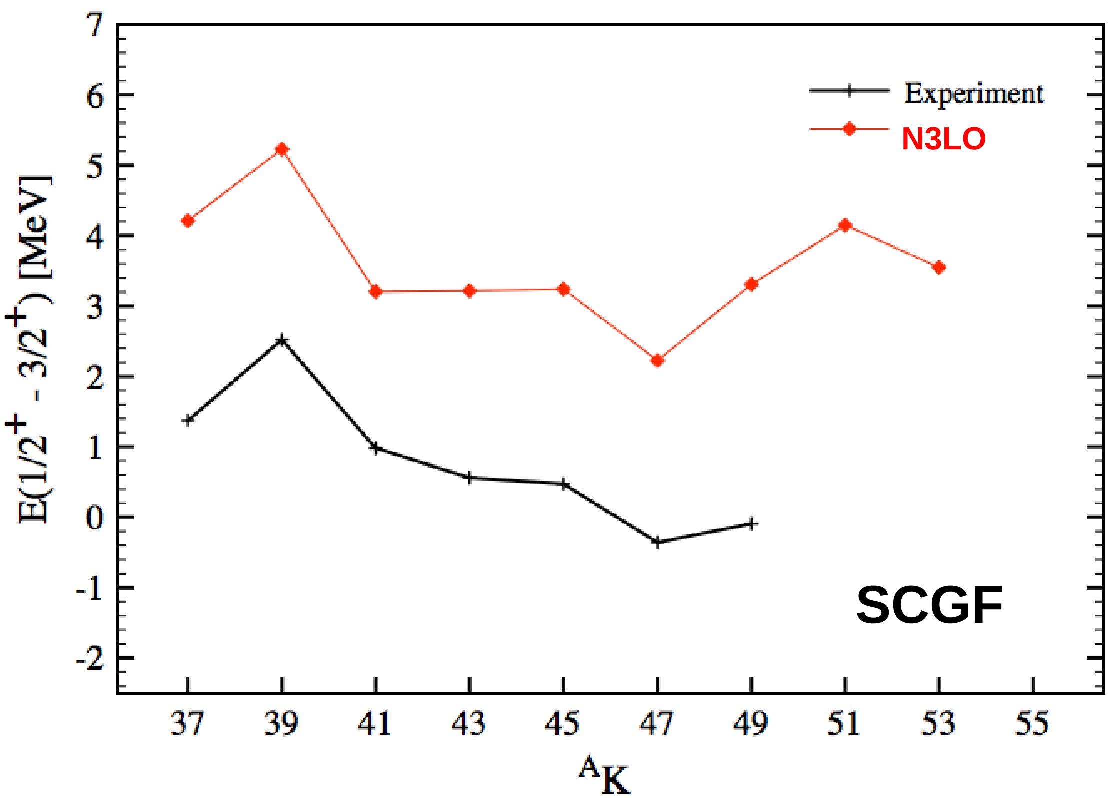
◉ **K spectra show interesting g.s. spin inversion and re-inversion**

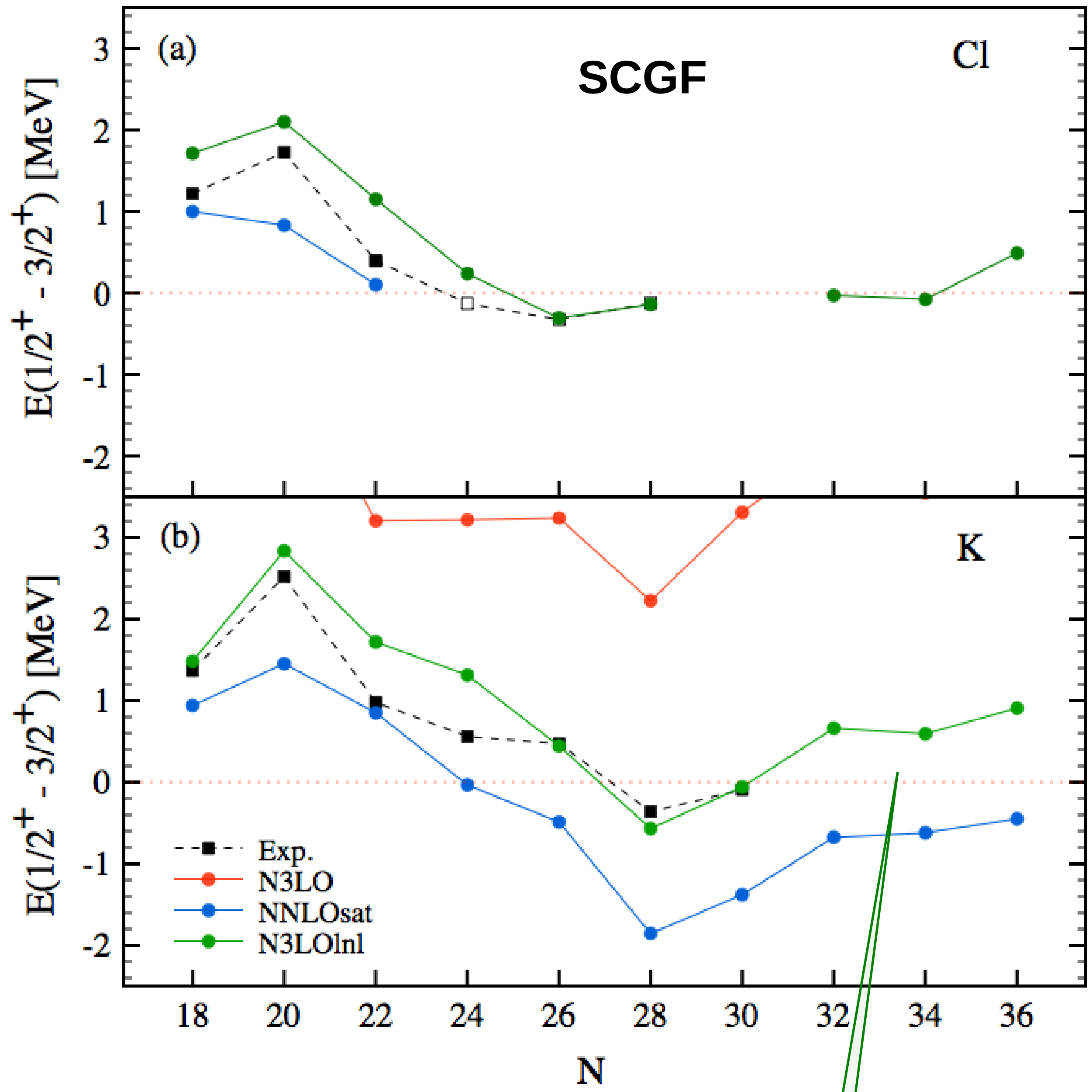
[Somà *et al.* 2019]

Laser spectroscopy COLLAPS @ ISOLDE



[Papuga *et al.* 2013]





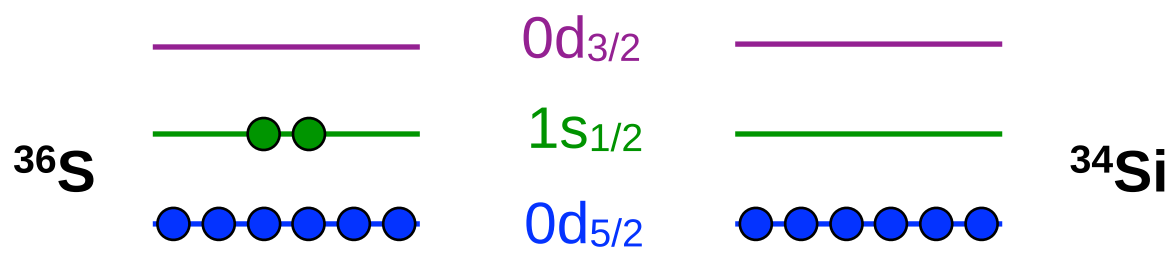
Recent experiment confirms N3LO$_{lnl}$ prediction for ^{51}K and ^{53}K

[Sun *et al.* in preparation]

Potential bubble nucleus ^{34}Si

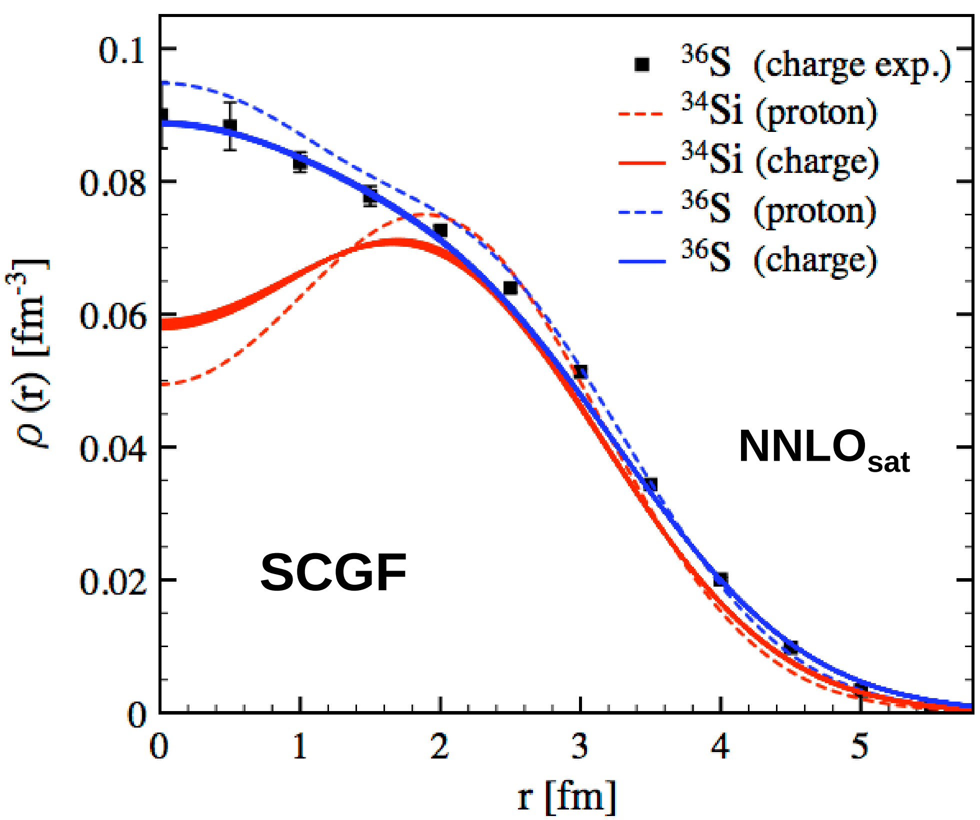
◉ Conjectured central depletion in $\rho_{ch}(r)$: **best candidate is ^{34}Si** [Todd-Rutel *et al.* 2004, Khan *et al.* 2008, …]

Naive proton filling



E_{2+} (^{34}Si)= 3.3MeV
[Ibbotson *et al.* 1998]

◉ **SCGF calculation with NNLO$_{sat}$ Hamiltonian** [Duguet *et al.* 2017]

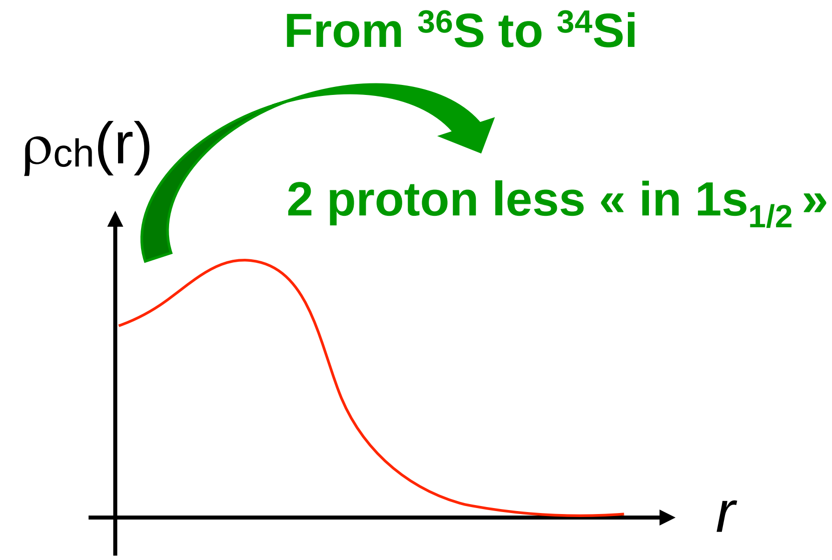


E	ADC(3)	Experiment
^{34}Si	−282.938	−283.427
^{36}S	−305.767	−308.714

1%

$\langle r^2_{ch}\rangle^{1/2}$	ADC(3)	Experiment
^{34}Si	3.187	
^{36}S	3.285	3.2985 ± 0.0024

0.5%



◉ **Depletion factor**

$$F \equiv \frac{\rho_{max} - \rho_c}{\rho_{max}}$$

^{34}Si	SCGF
F_p	0.34
F_{ch}	0.15

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

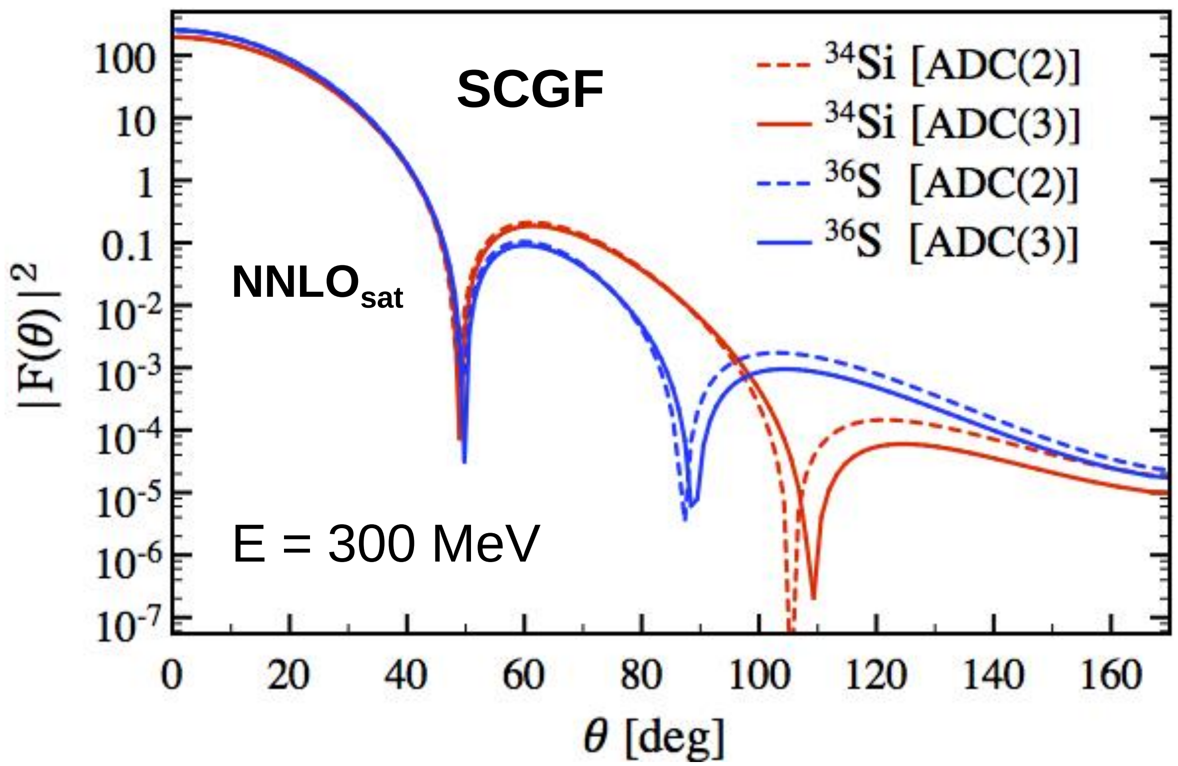
○ **Charge** density of ^{34}Si is predicted to display a **marked depletion in the center**

Charge form factor

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

PWBA

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



[Duguet *et al.* 2017]

LOI accepted

Nuclei	$T_{1/2}$	I^π	μ[nm]	Q[b]	$\langle r^2\rangle^{1/2}$ [fm]
^{24}Si	140 ms	0^+			
^{25}Si	220 ms	$5/2^+$			
^{26}Si	2.2 s	0^+			
^{27}Si	4.1 s	$5/2^+$	(-)0.8554(4)	(+)0.060(13)	
^{28}Si	stable	0^+			3.106(30)
^{29}Si	stable	$1/2^+$	-0.55529(3)		3.079(21)
^{30}Si	stable	0^+			3.193(13)
^{31}Si	157.3 m	$3/2^+$			
^{32}Si	153 y	0^+			
^{33}Si	6.1 s	$(3/2)^+$	(+)1.21(3)		
^{34}Si	2.8 s	0^+			
^{35}Si	0.8 s	$(7/2)^-$	(-)1.638(4)		

○ Central depletion reflects in larger $|F(\theta)|^2$ for **angles 60°<θ<90° and shifted 2nd minimum by 20°**

○ Visible in future **electron scattering** experiments **if enough luminosity** (10^{29} cm^{-2}s^{-1} for 2nd minimun)

○ Correlation between F_{ch} and $\langle r^2\rangle_{ch}^{1/2}$ (^{36}S) – $\langle r^2\rangle_{ch}^{1/2}$(^{34}Si) identified

■Measurement of **$\delta\langle r^2\rangle_{ch}^{1/2}$ (^{A}Si) from high-resolution laser spectroscopy@NSCL (R. Garcia-Ruiz)**

Addition and removal nucleon spectra

◉ Conjectured correlation between bubble and splitting between low *J* spin-orbit partners

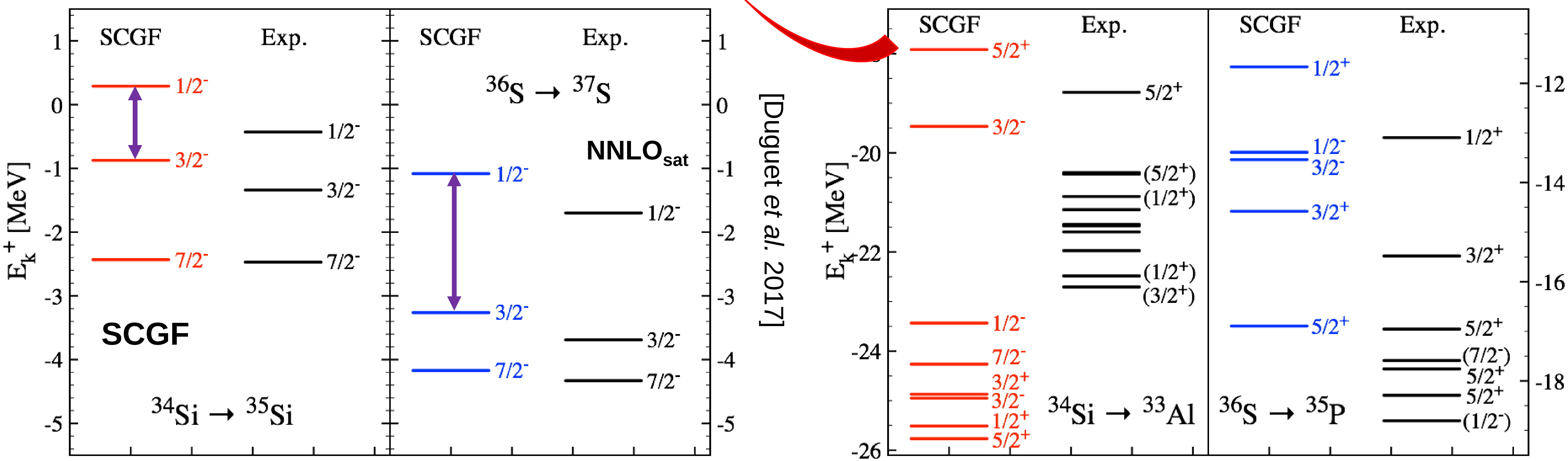
One-neutron addition

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

Quadrupole moment [Heylen *et al.* 2016]

One-proton knock-out

Exp. data: [Khan *et al.* 1985] [Mutschler *et al.* 2016] [Mutschler *et al.* 2017]



○ **Good agreement** for one-neutron addition to ^{35}Si and ^{37}Si (1/2$^-$ state in ^{35}Si needs continuum)

○ Much less good for one-proton removal; ^{33}Al on the edge of island of inversion: challenging!

○ **Correct reduction of splitting E$_{1/2^-}$ - E$_{3/2^-}$ from ^{37}S to ^{35}Si**

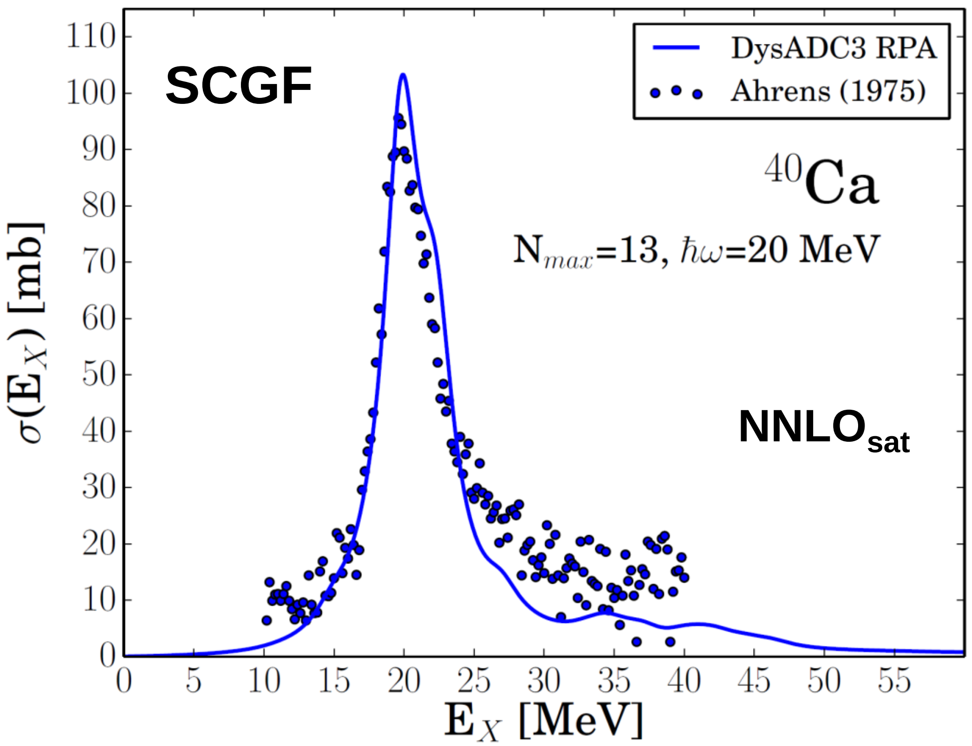
Such a sudden reduction of 50% is unique
Any correlation with the bubble? Yes!

$E_{1/2-} - E_{3/2-}$	^{37}S	^{35}Si	^{37}S→^{35}Si
SCGF	2.18	1.16	-1.02 (-47%)
(d,p)	1.99	0.91	-1.08 (-54%)

Electromagnetic response

◉ Photodisintegration cross section of ^{40}Ca

$$\sigma(E) \equiv 4\pi\alpha E R(E)$$



[Raimoni and Barbieri 2019]

Dipole response function

$$R(E) \equiv \sum_k |\langle \Psi_k | Q^{T=1}_{1m} | \Psi_0 \rangle| \delta(E_k - E_0 - E)$$

Electric dipole operator

$$Q^{T=1}_{1m} \equiv \frac{N}{N+Z} \sum_{p=1}^{Z} r_p Y_{1m}(\theta_p, \phi_p) - \frac{Z}{N+Z} \sum_{n=1}^{N} r_n Y_{1m}(\theta_n, \phi_n)$$

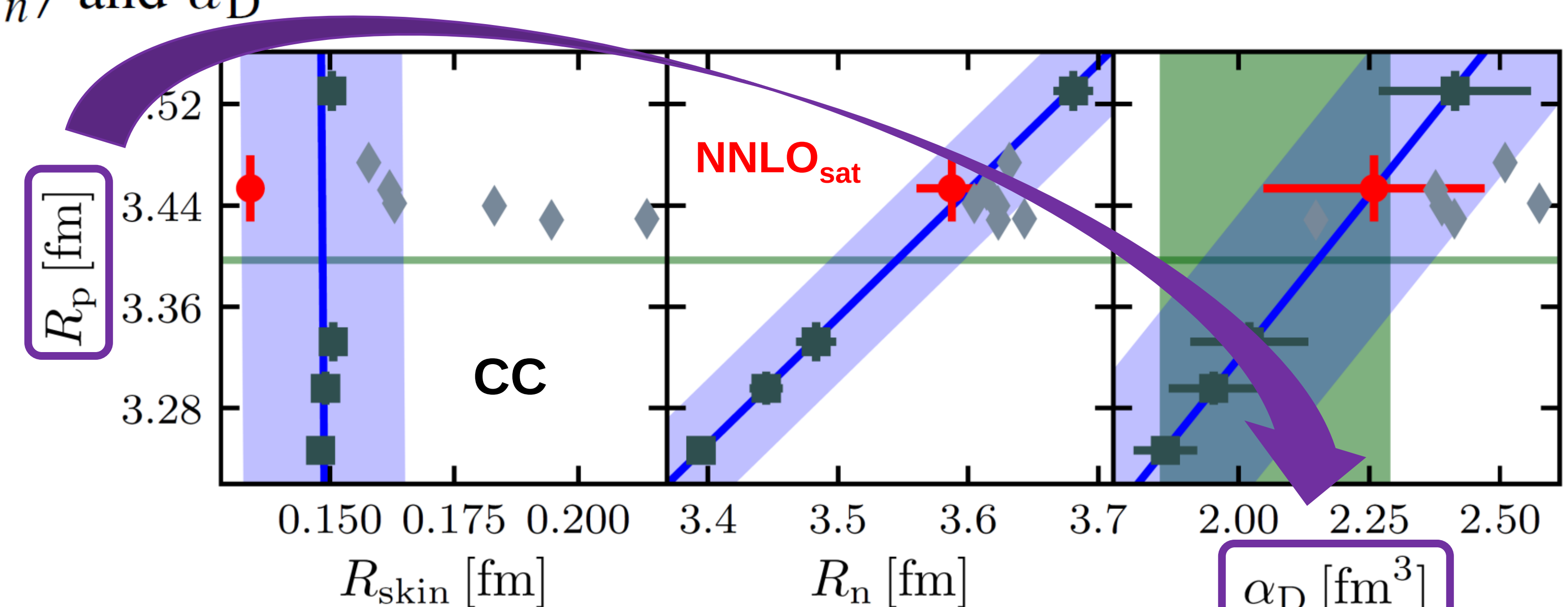
Giant and pygmy resonances accessible up to ^{A}Ni
Many-body correlations crucial for quantitative description

◉ Correlation between $\sqrt{\langle r_p^2 \rangle}$, $\sqrt{\langle r_n^2 \rangle}$ and α_D

Electric dipole polarizability

$$\alpha_D \equiv 2\alpha \int dE \frac{R(E)}{E}$$

$$\sqrt{\langle r^2_{ch} \rangle} \Longrightarrow \alpha_D$$



[Simonis *et al.* 2019]

Contents

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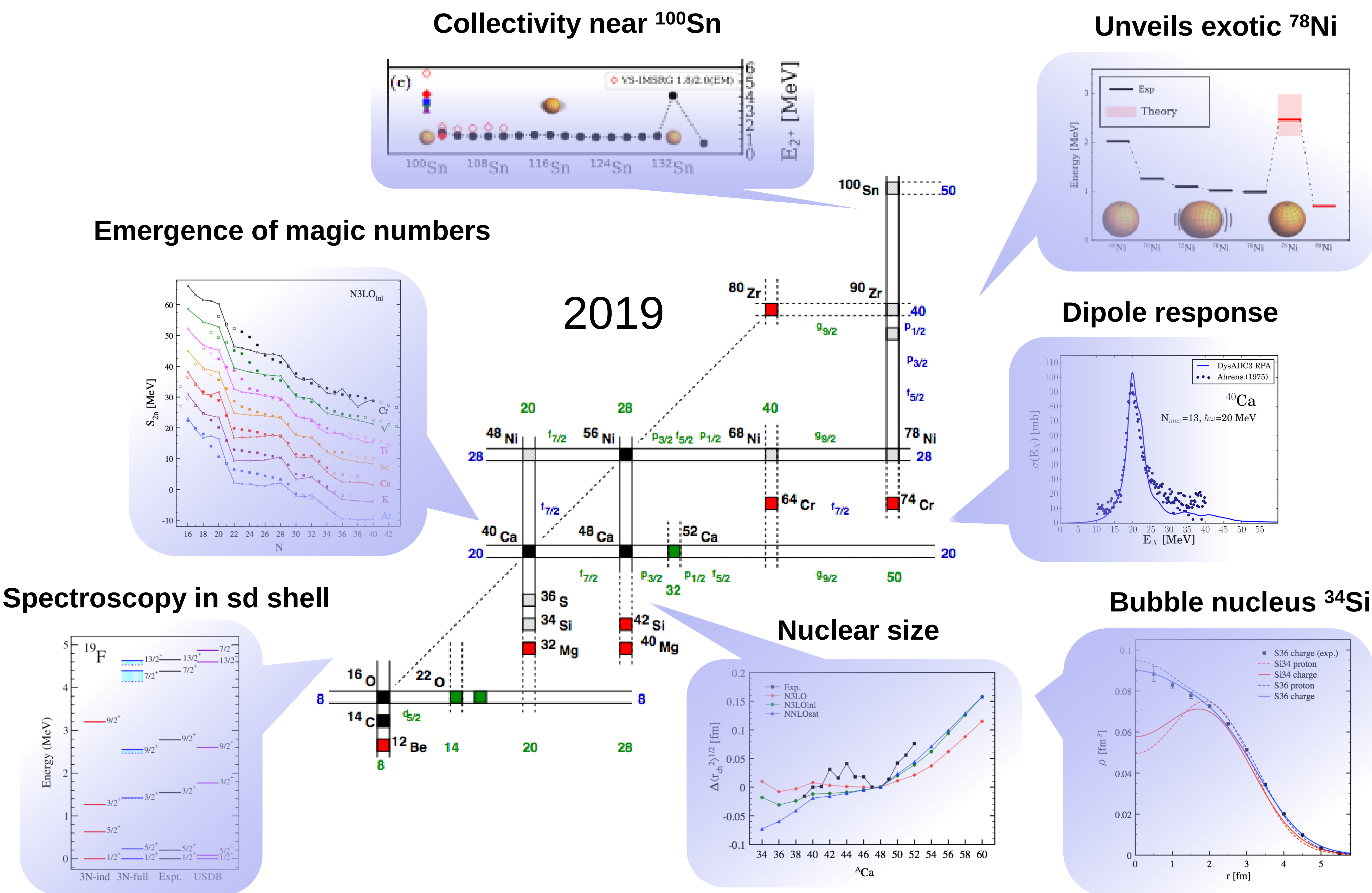
  - Definition and recent progress
  - Examples of recent applications
  - Some challenges and on-going developments
- Ab initio nuclear many-body problem and observables accessible via laser spectroscopy
  - Direct observables and indirect observables
  - Operators in chiral effective field theory
  - Applications in s and p shell nuclei
  - Applications in sd-pf shell nuclei
- Conclusions

Nuclear structure features addressed ab initio



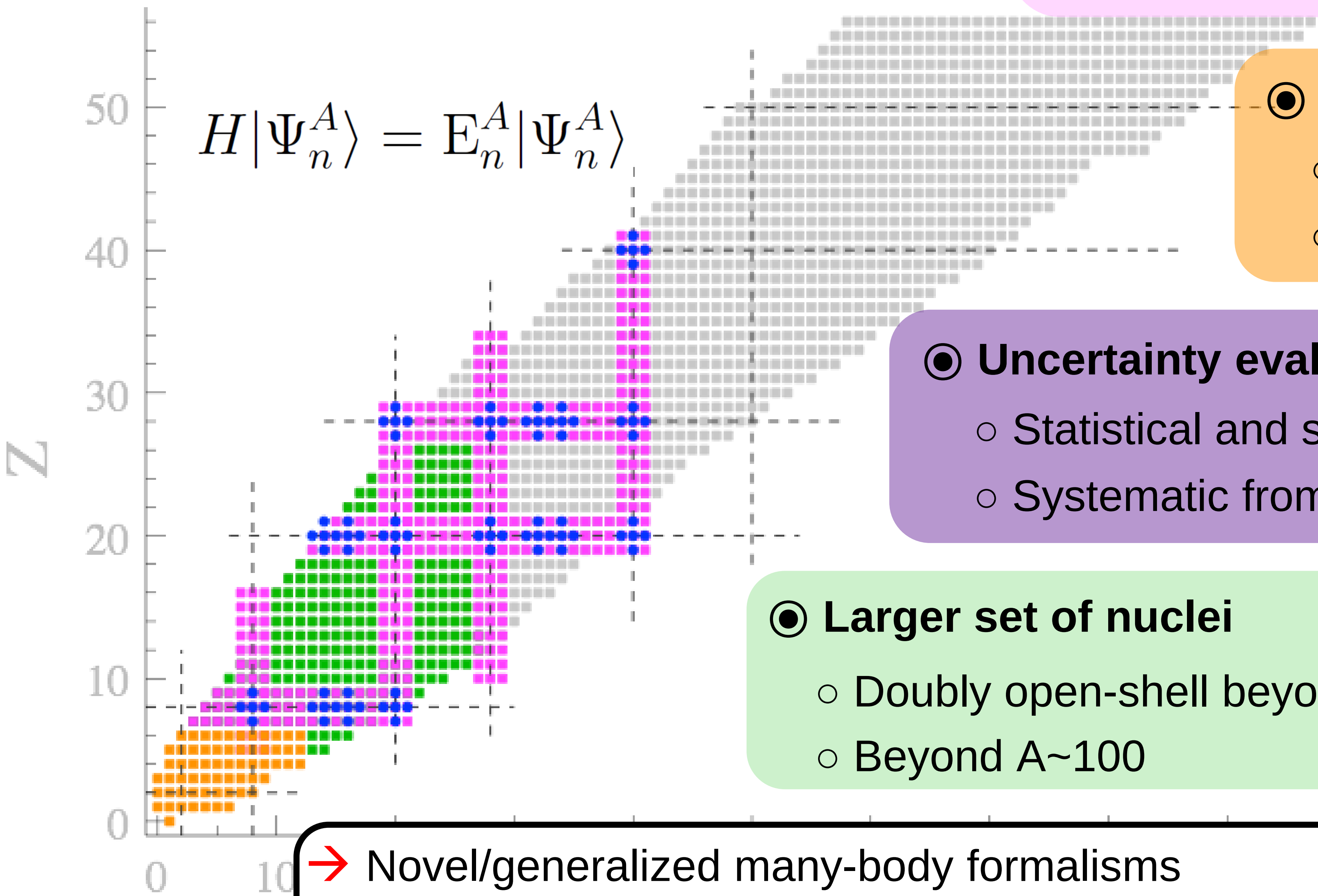
Some challenges for ab initio theory

◉ More accurate descriptions

- ○ Next order in expansion, e.g. full T3, pert. T4
- ○ Next order in H, e.g. full 3NF and approx 4NF

◉ Enlarged portefolio of observables

- ○ Low-lying E* in open-shell beyond sd
- ○ Moments in open-shell beyond sd
- ○ Giant resonances



◉ Improved Hamiltonians

- ○ Higher order, different fits
- ○ Different PW, Δ-full EFT

◉ Uncertainty evaluation/propagation

- ○ Statistical and systematic from H
- ○ Systematic from basis size, truncation order

◉ Larger set of nuclei

- ○ Doubly open-shell beyond sd shell
- ○ Beyond A~100

→ Novel/generalized many-body formalisms
→ Improved nuclear Hamiltonians
→ Data processing methods from applied mathematics

Contents

So what about observables from laser spectrocopy?

- **Charge radii via isotopic shifts**
  - Tremendously useful to tune bulk properties of nuclear interactions
  - **Now systematically computed for even-even closed and (singly) open-shell nuclei**
  - Entertain interesting correlations with other observables, e.g. α_D, F_{ch}…

- **Nuclear spins via atomic hyperfine structure**
  - Basic check of nuclear structure evolution
  - **Require the computation of odd-even or odd-odd ground-states/isomeric states**
  - Systematic comparison with available data could be useful

- **Ground-state electromagnetic moments via atomic hyperfine structure**
  - Detailed probe of nuclear structure evolution (« shell structure » and « shell occupancies »)
  - **Require the computation of odd-even or odd-odd ground-states**
  - **Require the computation of non-trivial operators**

Contents

Effective field theory

1. Use separation of scales to define d.o.f & expansion parameter [Weinberg, van Kolck, ..]

Typical momentum at play ← $\frac{Q}{M}$ → High energy scale (not included explicitly)

2. Parametrize physics beyond *M* + write all terms allowed by symmetries of underlying theory (QCD)

3. Order by size all possible terms → systematic expansion ("power counting") → theoretical error

4. Truncate at a given order and adjust low-energy constants (LECs) via underlying theory or data

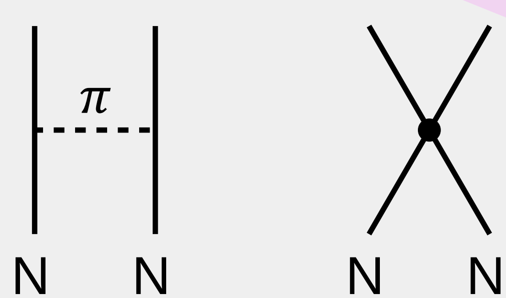
5. Regularize UV divergences and (hopefully) achieve order-by-order renormalization of observables

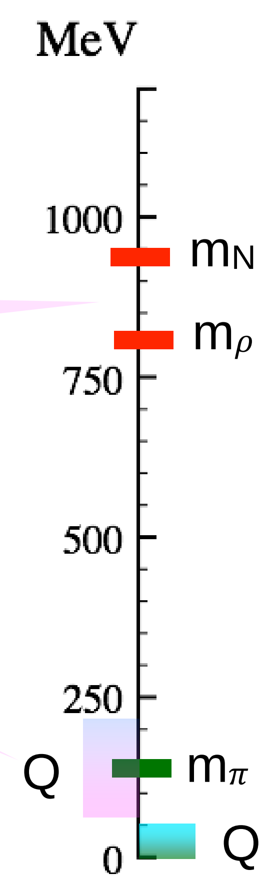
Chiral EFT

➪ Expand around $Q \sim m_\pi$

High-energy via contact interactions

Keep pion dynamic explicit

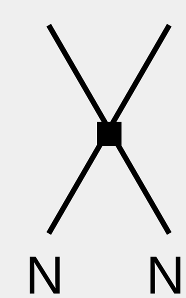




Pionless EFT

➪ Expand around Q ~ 0

Integrate out pions too
→ only contact terms

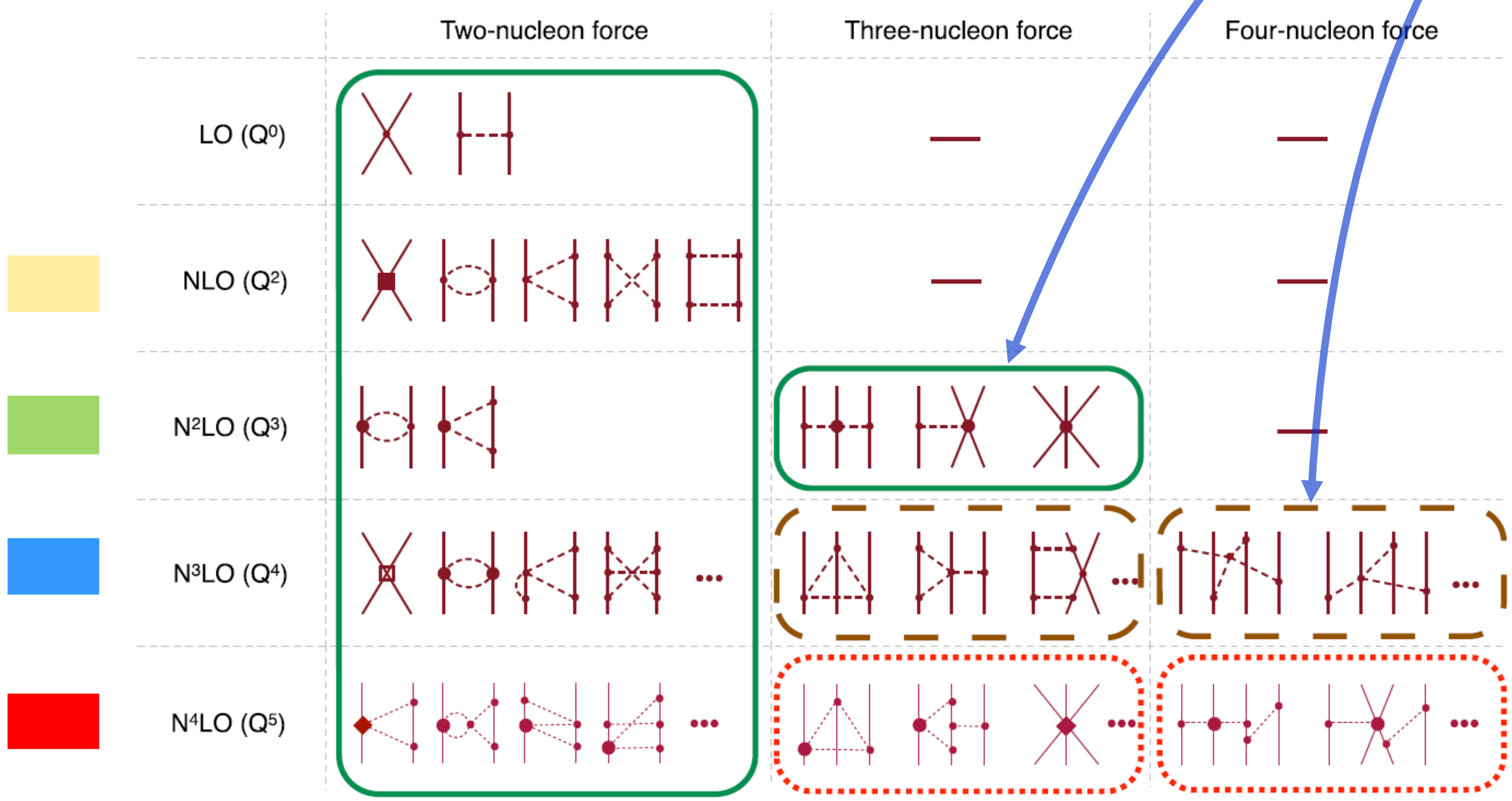


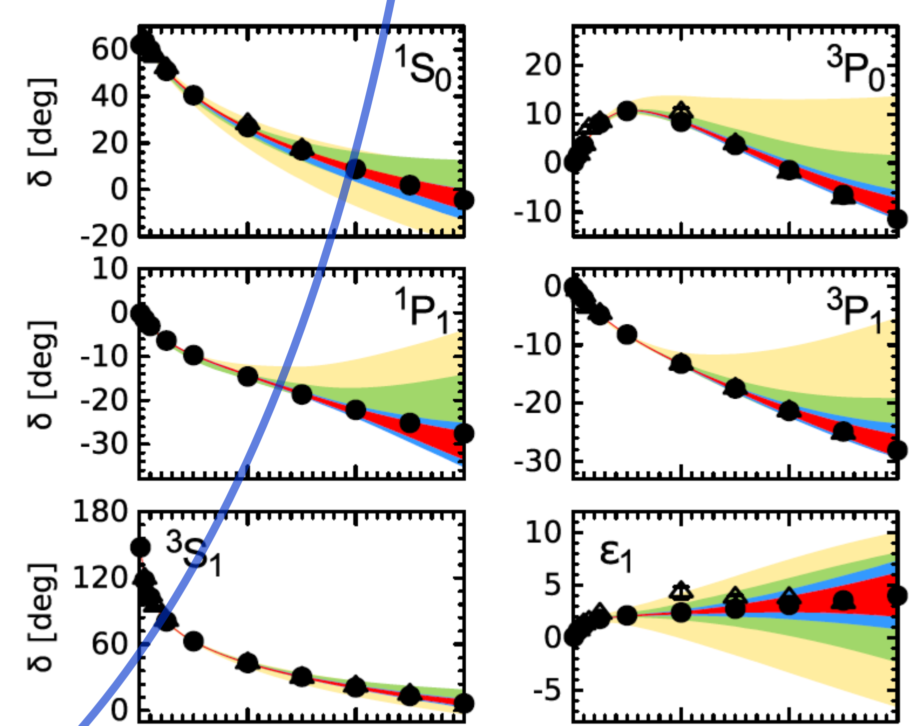
Hamiltonian in chiral effective field theory

- Hamiltonian $H = \sum_i t_i + \sum_{i<j} v_{ij} + \sum_{i<j<k} w_{ijk} + \ldots$ to be fed into $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$
- Consistent modeling of 2N, 3N, 4N… AN interactions
- Is the chiral expansion converging quickly enough?
  → If not, the approach becomes untractable

3N, 4N… appear at subleading orders

Can *k*N interactions beyond *k*=3 be omitted in *A*N systems with A>>3?





[Meißner 2016]

- Goal of **many**-body methods: apply to *A*N systems with ***A>>3*** (and propagate the theoretical error!)

Consistent operators in chiral effective field theory

✓ **Nuclear electromagnetic charge/current operators** **(= time/vector part of four-vector current j^μ)**

$$\rho(\vec{q}) = \sum_i \rho_i(\vec{q}) + \sum_{i<j} \rho_{ij}(\vec{q}) + \sum_{i<j<k} \rho_{ijk}(\vec{q}) + \ldots$$

$$\vec{j}(\vec{q}) = \sum_i \vec{j}_i(\vec{q}) + \sum_{i<j} \vec{j}_{ij}(\vec{q}) + \sum_{i<j<k} \vec{j}_{ijk}(\vec{q}) + \ldots$$

◉ **One-body (i.e. standard) operator**

◉ **Two-body meson-exchange currents (MECs)**

◉ **Three-body meson-exchange currents**

⋮

$\vec{q}$ = momentum of external photon field

◉ Operators are built from EFT expansion by coupling nuclear current to external e.m. fields

○ **Consistent nuclear e.m. operators and nuclear forces**

○ Satisfy the continuity equation $\vec{q}.\vec{j}(\vec{q}) = [H, \rho(\vec{q})]$ following from gauge invariance

○ Derived via two different version of time-ordered perturbation theory

- Standard time-ordered perturbation theory / Jlab-Pisa group [Pastore et al. 2008, 2009, 2011, 2013]
- Method of unitary transformation / Bochum-Bonn group [Kolling et al. 2009, 2011]

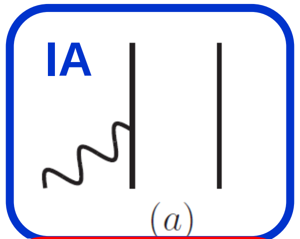
→ Proper renormalization achieved in this case

Electromagnetic current operator

One-body current ↔ NR expansion of covariant single-nucleon current operator
↔ simplified picture that e.m. properties due to free nucleons

$$\vec{K}_i = (\vec{p}\,'_i + \vec{p}_i)/2 \qquad \vec{k}_i = \vec{p}\,'_i - \vec{p}_i \qquad Q^2_\mu = q^2 - \omega^2$$

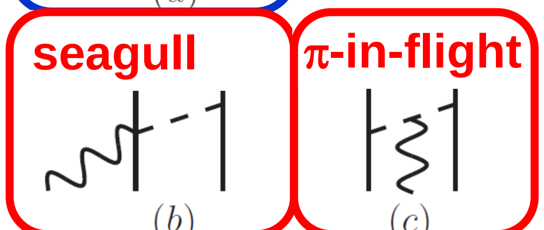
LO $e\,Q^{(-2)}$



$$\vec{j}^{\,\rm LO}_i(\vec{K}_i,\vec{k}_i;\vec{q}) = \frac{e}{2m}\left[2e_i(Q^2_\mu)\vec{K}_i + i\mu_i(Q^2_\mu)\vec{\sigma}_i\times\vec{q}\right]\delta(\vec{k}_i - \vec{q})$$

convection — spin magnetization

NLO $e\,Q^{(-1)}$

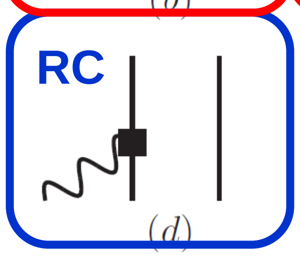


$$\vec{j}^{\,\rm NLO}_{ij}(\vec{k}_i,\vec{k}_j;\vec{q}) = -ie\frac{g_A^2}{F_\pi^2}(\vec{\tau}_i\times\vec{\tau}_j)^z\left(\vec{\sigma}_i - \vec{k}_i\frac{\vec{\sigma}_i.\vec{k}_i}{k_i^2+m_\pi^2}\right)\frac{\vec{\sigma}_j.\vec{k}_j}{k_j^2+m_\pi^2} + i \rightleftarrows j$$

Strict chiral expansion does not converge (fast enough)
→Account of nucleonic e.m. structure via form factor

Two-body current ↔ current from exchanged pions
↔ associated with OPE in 2NF - IV

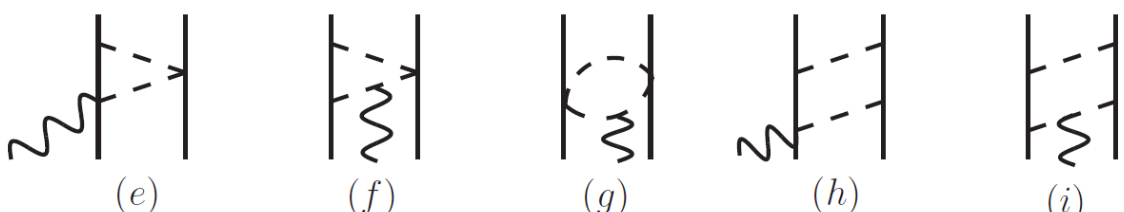
N²LO $e\,Q^{(0)}$



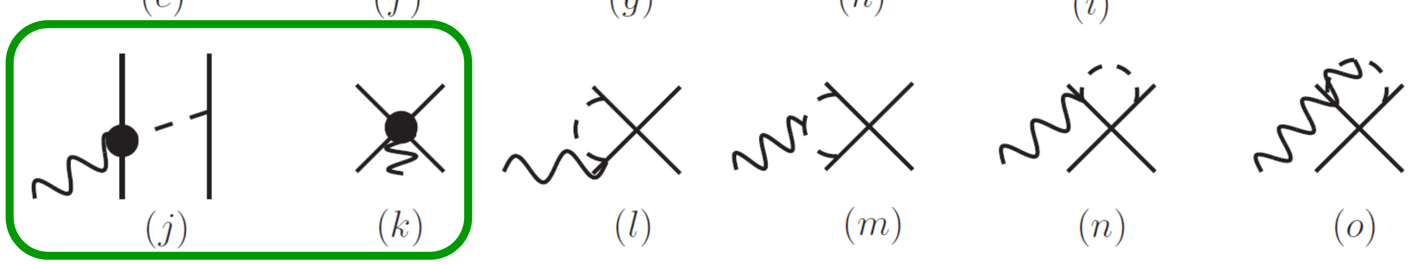
Suppressed by $(Q/m)^2$

Full N³LO current satisfies continuity equation
Three-body MECs enter at N⁴LO (not derived yet)

N³LO $e\,Q^{(1)}$



↔ One-loop TPE [(e)-(i)] - IV
↔ One-loop OPE-CT [(l)-(o)] - IV
↔ CT [(k)] - IV+IS



3 « minimal » LECs from OPE (j)
2 « non-minimal » LECs from CT (k)

Operator	LO	NLO	N2LO	N3LO	N4LO
j	$\nu = -2$ IA(NR)	$\nu = -1$ OPE	$\nu = 0$ IA(RC)	$\nu = 1$ OPE(LECs) TPE CT(LECs)	

Nucleon's electric/magnetic form factors

$$e_i(Q^2_\mu) = \frac{G^S_E(Q^2_\mu) + G^V_E(Q^2_\mu)\tau^z_i}{2}$$

$$\mu_i(Q^2_\mu) = \frac{G^S_M(Q^2_\mu) + G^V_M(Q^2_\mu)\tau^z_i}{2}$$

$$G^S_E(0) = G^V_E(0) = 1$$

$$G^S_M(0) = 0.880\mu_N$$

$$G^V_M(0) = 4.706\mu_N$$

Electromagnetic charge operator

One-body charge ↔ NR expansion of covariant single-nucleon current operator
↔ simplified picture that e.m. properties due to free nucleons

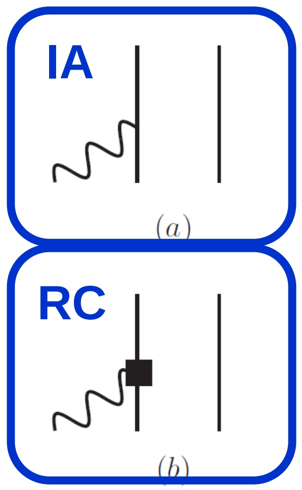
$\vec{K}_i = (\vec{p}\,'_i + \vec{p}_i)/2$

$\vec{k}_i = \vec{p}\,'_i - \vec{p}_i$

$Q^2_\mu = q^2 - \omega^2$

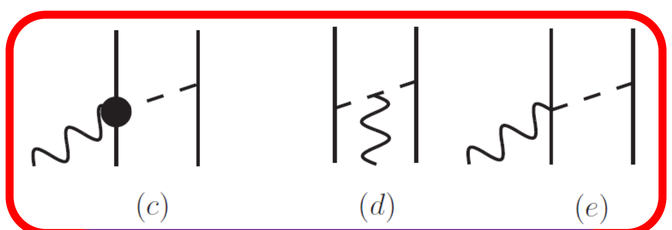
LO $e\,Q^{(-3)}$

N²LO $e\,Q^{(-1)}$

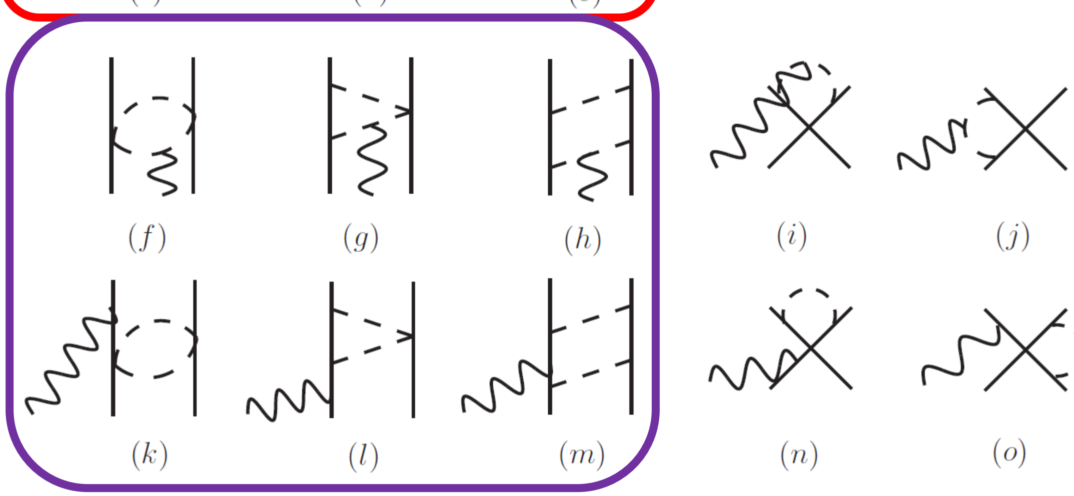


$$\rho_i^{\mathrm{LO}}(\vec{k}_i;\vec{q}) = e\, e_i(Q^2_\mu)\,\delta(\vec{k}_i - \vec{q})$$

N³LO $e\,Q^{(0)}$



N⁴LO $e\,Q^{(1)}$



Structure of charge and current operators differ significantly

↔ j^{LO} suppressed by one factor of Q compared to ρ^{LO}

↔ NLO OPE contributions to ρ vanish in static limit

↔ Two-body OPE MECs enter j/ρ at NLO/N³LO

↔ Two-body TPE MECs enter j/ρ at N³LO/N⁴LO

↔ **ρ does not involved unknowns LECs**

↔ **Three-body MECs enter ρ at Q (i.e. N4LO, not shown here)**

Operator	LO	NLO	N2LO	N3LO	N4LO
ρ	$\nu = -3$ IA(NR)	$\nu = -2$ —	$\nu = -1$ IA(RC)	$\nu = 0$ OPE	$\nu = 1$ TPE

Nucleon's electric/magnetic form factors

$$e_i(Q^2_\mu) = \frac{G^S_E(Q^2_\mu) + G^V_E(Q^2_\mu)\tau^z_i}{2}$$

$$\mu_i(Q^2_\mu) = \frac{G^S_M(Q^2_\mu) + G^V_M(Q^2_\mu)\tau^z_i}{2}$$

$G^S_E(0) = G^V_E(0) = 1$

$G^S_M(0) = 0.880\mu_N$

$G^V_M(0) = 4.706\mu_N$

Relation to observables from laser spectroscopy

- Longitudinal and transverse form factors for elastic and inelastic scattering

$$F_L^2(q) = \frac{1}{2J_i+1}\sum_{J=0}^{\infty} |\langle \Psi_f^{J_f} | T_J^C(q) | \Psi_i^{J_i}\rangle|^2$$

$T^C_J \leftarrow$ multipole expansion of ρ

$$F_T^2(q) = \frac{1}{2J_i+1}\sum_{J=0}^{\infty} |\langle \Psi_f^{J_f} | T_J^M(q) | \Psi_i^{J_i}\rangle|^2 + |\langle \Psi_f^{J_f} | T_J^E(q) | \Psi_i^{J_i}\rangle|^2$$

T^M_J and $T^E_J \leftarrow$ multipole expansion of j

- Connection to static moments

→ Elastic scattering on ground-state: $J_i = J_f = J_0$
→ Static limit: q = 0

$$T_2^C(0) \propto Q$$

$$T_1^M(0) \propto \mu$$

- Form of standard one-body, i.e. LO(IA), operators

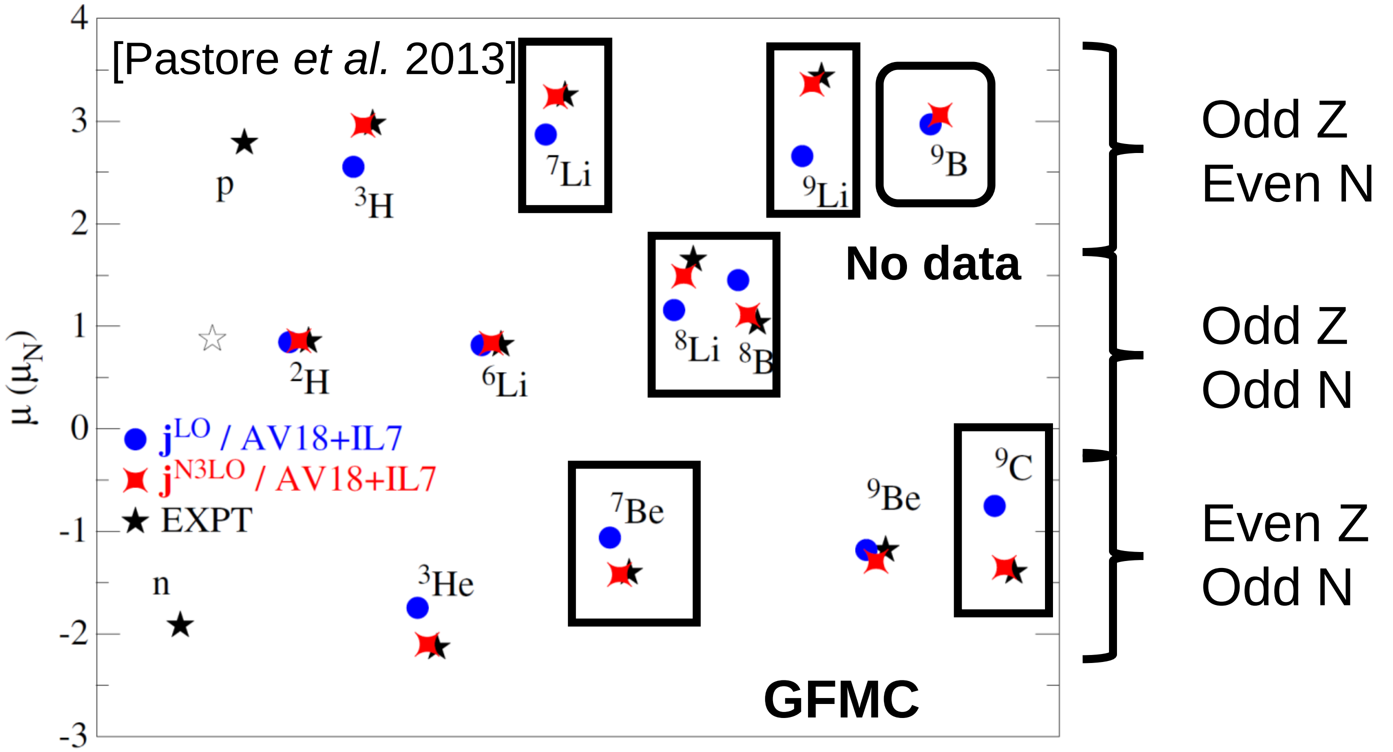
  - Static electric quadrupole operator $$Q^{\mathrm{IA}} = e\sum_i e_i(0)\, r_i^2\, Y_{20}(\theta_i,\phi_i)$$

  - Static magnetic dipole operator $$\mu^{\mathrm{IA}} = \sum_i e_i(0)\,\vec{L}_i + \mu_i(0)\,\vec{\sigma}_i$$

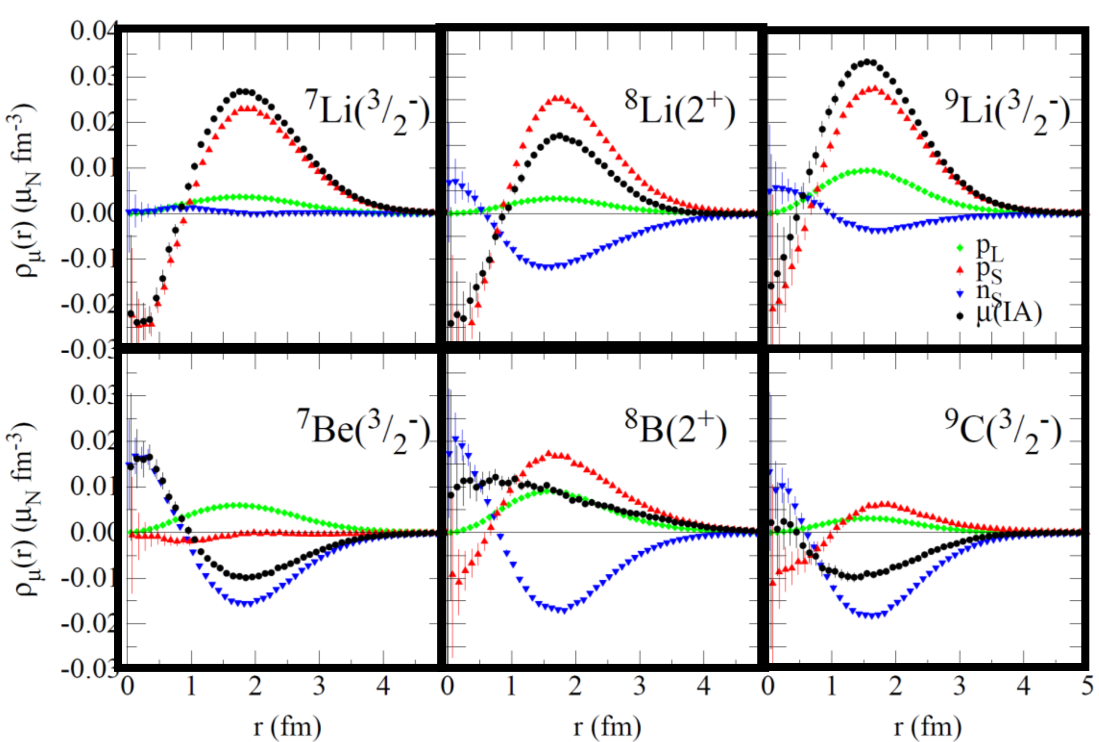
Contents

Magnetic dipole moment in s and p shell nuclei

◉ (Hybrid) calculations with e.m. currents from χ-EFT



◉ Magnetic densities



◉ **Dipole operator**

- LO (IA) and up to N^{3}LO
- Nucleon form factors
- **LECs adjusted on μ of A=2,3**

◉ **Dipole moment**

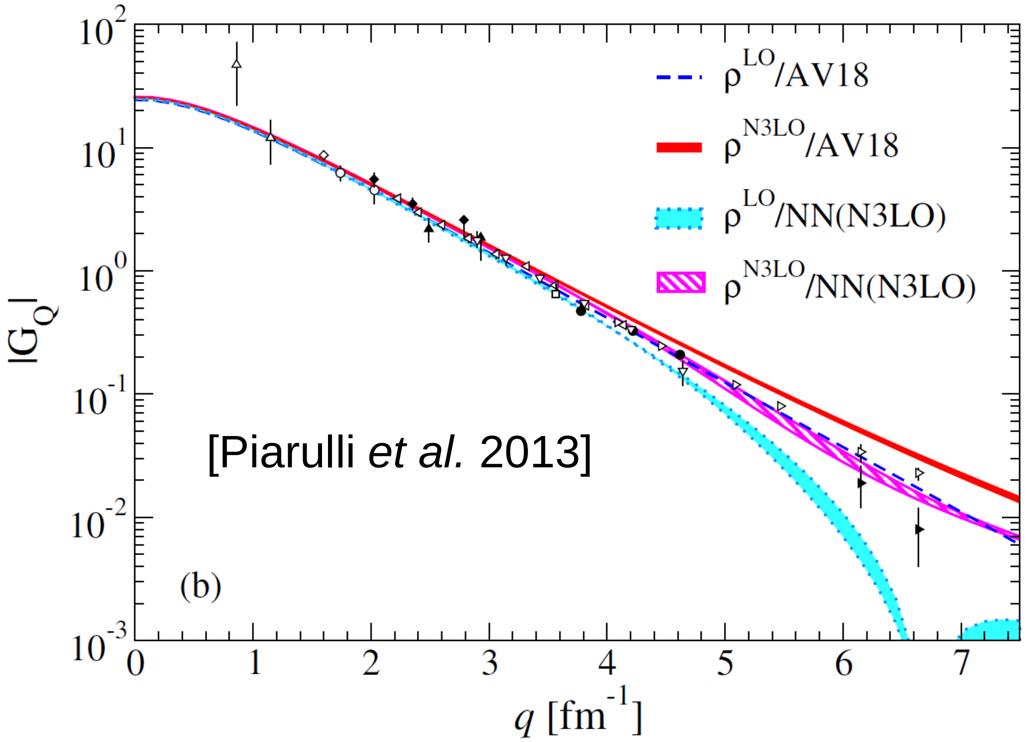
- Excellent account of data
- Dominated by one-body (IA)
- **Two-body MEC up to 40%**
- MEC (almost) always improve

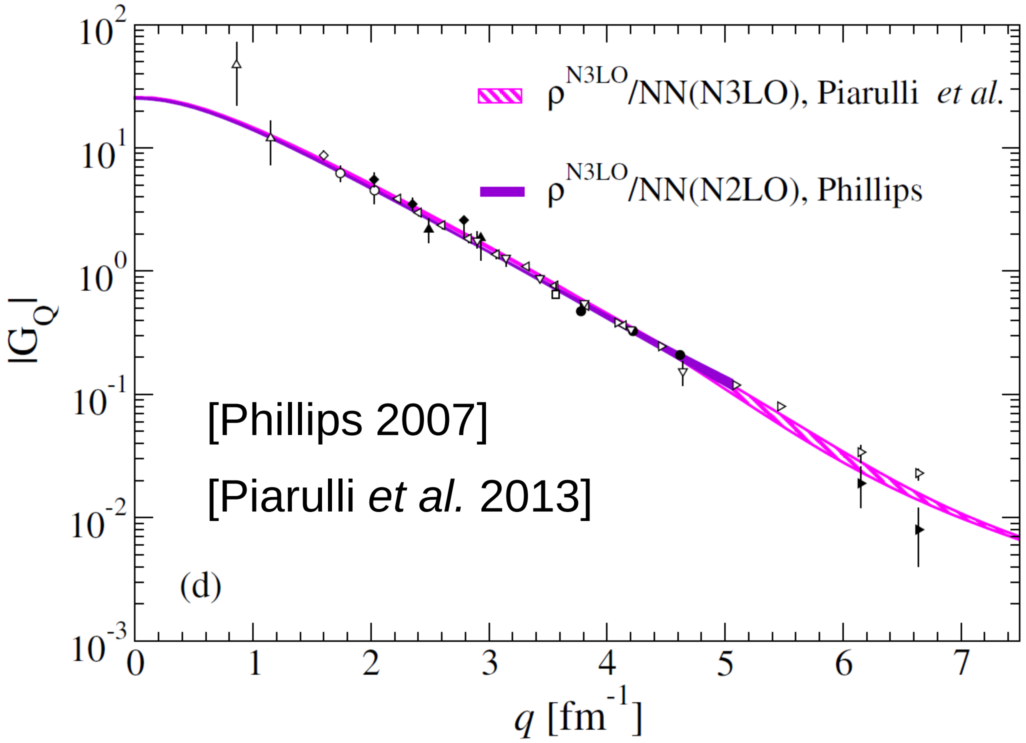
◉ **Decomposition of one-body IA**

- Proton's convection small vs spin magnetization
- **Driven by valence nucleon in odd-even**
- **Driven by n-p or 3He-p cluster in odd-odd**

Elastic form factors in s and p shell nuclei

◉ Elastic charge (longitudinal) and magnetic (transverse) form factors from ^{2}H to ^{12}C





◉ Ex: Quadrupole electric form factor in ^{2}H

- ○ Hybrid and (semi-consistent) χ-EFT calculations
- ○ **Charge operator at LO (IA) and N^3LO**
- ○ Band from 500 MeV < Λ < 600 MeV

◉ Results

- ○ **$G_Q(0) = M^2_d\ Q_d$ (here in fit of NN)**
- ○ LO(IA) sufficient up to q~3 fm-1
- ○ Nucleonic form factors mandatory beyond 1.5 fm^{-1}
- ○ Excellent result up to q ~ 4 fm^{-1} in all cases
- ○ **χ-EFT with N^3LO MEC excellent up to q ~ 8 fm^{-1}**

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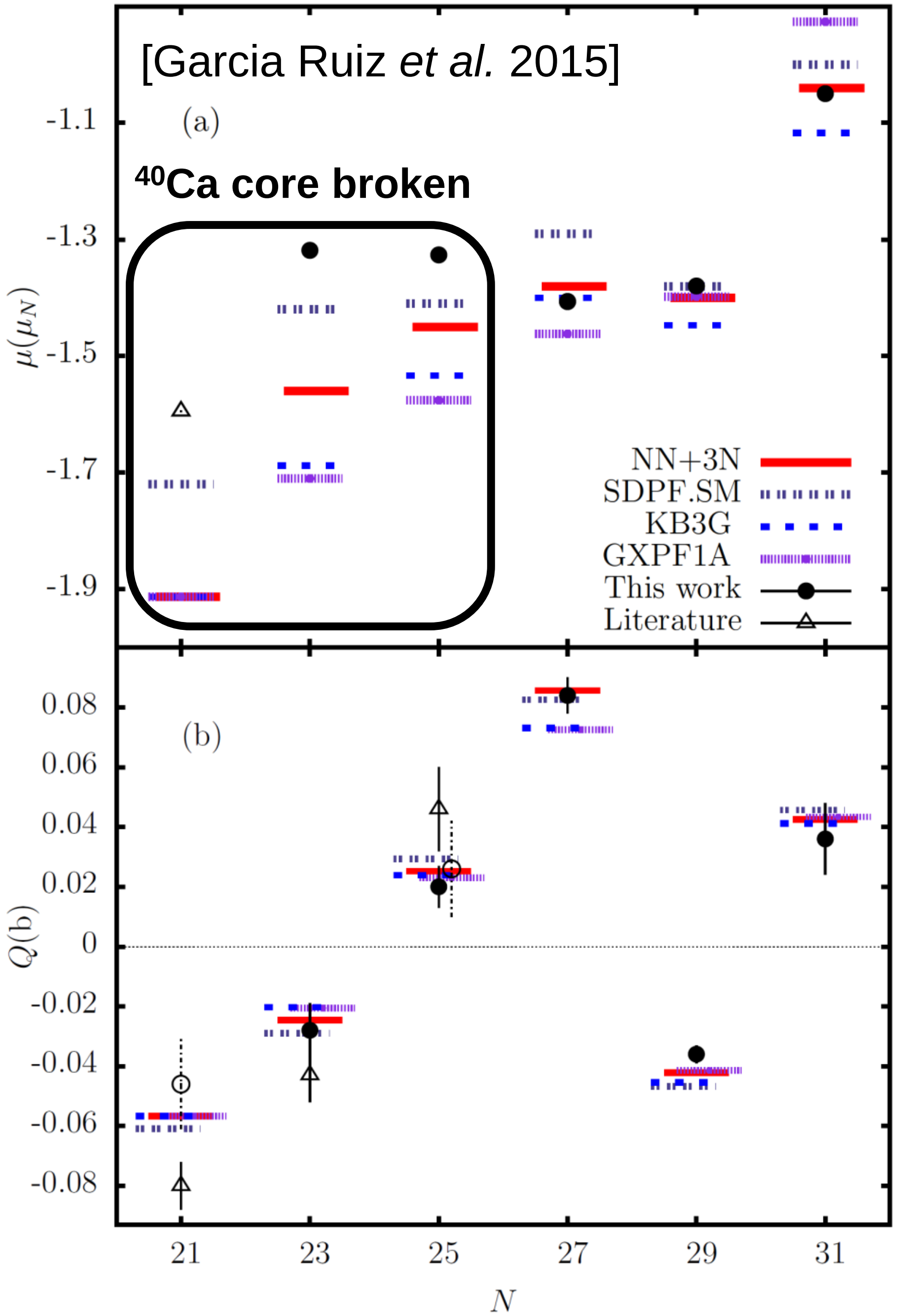
Moments in Ca isotopes

◉ Empirical/ab initio (IMSRG) shell-model calculations of magnetic dipole/electric quadrupole moments

- **^{47,49,51}Ca via high-resolution collinear laser spectroscopy COLLAPS @ ISOLDE [Garcia Ruiz *et al.* 2015]**
- ^{37}Ca via collinear laser spectroscopy BECOLA @ NSCL [Klose *et al.* 2019]



◉ Operators

- ○ Pure one-body ↔ No explicit MEC
- ○ Bare spin and orbital g factors for magnetic moment
- ○ Effective charges: e_n = 0.5e and e_p = 1.5e

◉ Magnetic moment

- ○ ^{40}Ca core broken in ^{41,43,45}Ca
- ○ **Good reproduction from ab initio in ^{47,49,51}Ca**
- ○ Significant breaking of N=32 magic number

◉ Quadrupole moment

- ○ **Excellent agreement for ab initio in all isotopes**
- ○ No apparent need of orbital-dependent e_n and/or e_p

Next: MEC and consistently-transformed operators to valence space

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Conclusions

◉ **Enormous progress of ab initio calculations in the last 10 years**

- ○ Much larger phenomenology can be put in connection with elementary nuclear forces
- ○ Nuclear forces themselves are explicitly rooted in QCD
- ○ Comparison to basic experimental observables can be made to day up to $A \approx 80$

◉ **Much further progress to be made**

- ○ Observables: electromagnatic moments and transitions, electroweak operators
- ○ Nuclear interactions put to the test in mid-mass nuclei = current main bottleneck for progress
- ○ Formal & numerical challenges to go to heavier nuclei/better accuracy/doubly open-shell nuclei
- ○ Compute features of reactions (already some) and develop ab initio dynamics
- ○ Evaluation and propagation of systematic errors of H

Collaborators on ab initio many-body calculations

J.-P. Ebran
M. Frosini
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V. Somà
A. Tichai

P. Arthuis
C. Barbieri
M. Drissi

G. Hagen
T. Papenbrock

D. Lacroix

P. Navratil

R. Roth

P. Demol

Back up slides

Hamiltonian

Nuclear Hamiltonian

$$H \equiv \frac{1}{(1!)^2}\sum_{pq} t_{pq} c^\dagger_p c_q + \frac{1}{(2!)^2}\sum_{pqrs} \bar{v}_{pqrs} c^\dagger_p c^\dagger_q c_s c_r + \frac{1}{(3!)^2}\sum_{pqrstu} \bar{w}_{pqrstu} c^\dagger_p c^\dagger_q c^\dagger_r c_u c_t c_s$$

} Genuine 3N interaction / six-legs vertex

Particle number

$$A \equiv \sum_p c^\dagger_p c_p$$

k-body force
↕
Mode-2k tensor
↕
Basis representation dim N
↕
Storage cost N^{2k}

Problematic to handle 3N interactions in mid-mass nuclei

Grand potential

$$\Omega \equiv H - \lambda A$$

When working in Fock space

Chemical potential

Controls the average particle number in the system

Single-reference expansion many-body methods

Nuclear Hamiltonian

$$H = T + V^{2N} + W^{3N}$$

Symmetry group

U(1) dealt with today

$[H, S] = 0$ where $S \equiv A, J^2, J_z \dots$

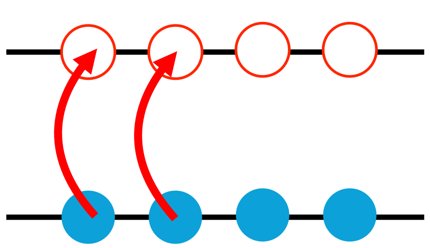
Mean-field reference state

$H = H_0 + H_1$ such that $[H_0, S] = 0$, $[H_1, S] = 0$

$$H_0|\Phi_0^S\rangle = \mathcal{E}_0^S|\Phi_0^S\rangle$$

Exactly solvable

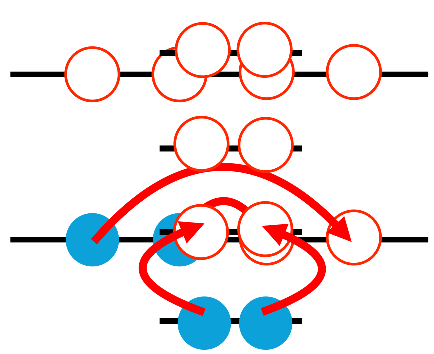
Closed-shell



Non-degenerate

Good starting point

Open-shell



Non-degenerate

Degenerate

Proper starting point

Improper starting point

A-body eigenvalue problem

$H|\Psi_0^S\rangle = E_0^S|\Psi_0^S\rangle$ N^A cost where N = dim $\mathcal{H}_1$

Many-body expansion

$$H = H_0 + H_1$$

$$|\Psi_0^S\rangle = U^S(\infty)|\Phi_0^S\rangle$$

Wave operator Reference state

▶ Accounts for « weak/dynamical » correlations

▶ Expand as a series (MBPT, CC…) + truncate = N^p cost

Symmetry breaking

$[H'_0, S] \neq 0$

$[H'_1, S] \neq 0$

$$H = H'_0 + H'_1$$

$$|\Psi_0^S\rangle = U(\infty)|\Phi_0\rangle$$

More general reference state

▶ Accounts for "strong/non-dynamical" correlations

▶ Expand (BMBPT, BCC…) + truncate = N^p cost

1) Truncated series breaks symmetry

2) Exact symmetry must eventually be restored

Slater determinant reference state and normal ordering

Slater determinant reference state

$$a_q^\dagger = \sum_p U_{pq}\, c_p^\dagger \qquad |\Phi^A\rangle \equiv \prod_{i=1}^{A} a_i^\dagger |0\rangle$$

Particle states a,b,c…

Hole states i,j,k…

Typically obtained by solving HF

Respect U(1) symmetry

$$A|\Phi^A\rangle = \mathrm{A}|\Phi^A\rangle$$

Normal ordering via Wick's theorem in single-particle basis

$$H \equiv \Lambda^{00} + \frac{1}{1!1!}\sum_{l_1 l_2} \Lambda^{11}_{l_1 l_2} : c^\dagger_{l_1} c_{l_2} : + \frac{1}{2!2!}\sum_{l_1 l_2 l_3 l_4} \Lambda^{22}_{l_1 l_2 l_3 l_4} : c^\dagger_{l_1} c^\dagger_{l_2} c_{l_4} c_{l_3} :$$

$$+ \frac{1}{3!3!}\sum_{l_1 l_2 l_3 l_4 l_5 l_6} \Lambda^{33}_{l_1 l_2 l_3 l_4 l_5 l_6} : c^\dagger_{l_1} c^\dagger_{l_2} c^\dagger_{l_3} c_{l_6} c_{l_5} c_{l_4} :$$

Anti-symmetric fields Λ^{ij} function of

$$t_{pq} \quad \overline{v}_{pqrs} \quad \overline{w}_{pqrstu} \quad U_{pk}$$

Similarly for *A* and Ω

Six-index tensor
Too expensive to handle

NO2B approximation
1-3% error in closed shell
[R. Roth *et al.*, PRL 109 (2012) 052501]

Effective 2-body operators
Captures essential of 3-body
Many-body method with 2-body

Bogoliubov reference state and normal ordering

Bogoliubov reference state

Breaks U(1) symmetry

$$\beta_k = \sum_p U^*_{pk} c_p + V^*_{pk} c^\dagger_p$$

$$\beta^\dagger_k = \sum_p U_{pk} c^\dagger_p + V_{pk} c_p$$

$$|\Phi\rangle \equiv C \prod_k \beta_k |0\rangle$$

$$\beta_k |\Phi\rangle = 0 \;\; \forall k$$

$$A|\Phi\rangle \neq \mathrm{A}|\Phi\rangle$$

Vacuum state
Reduces to SD in $\mathcal{H}_A$ for closed-shell

Normal ordering via Wick's theorem in quasi-particle basis

$$H \equiv \sum_{n=0}^{3} \sum_{i+j=2n} \frac{1}{i!\,j!} \sum_{l_1 \dots l_{i+j}} H^{ij}_{l_1 \dots l_{i+j}} \beta^\dagger_{k_1} \dots \beta^\dagger_{k_i} \beta_{k_{i+j}} \dots \beta_{k_{i+1}}$$

$$\equiv \underbrace{H^{00} + [H^{20} + H^{11} + H^{02}]}_{H_0} + [H^{40} + H^{31} + H^{22} + H^{13} + H^{04}] + \sum_{i+j=6} H^{ij}$$

$$\equiv \sum_{n=0}^{2} H^{[2n]} + H^{[6]}$$

6-qp operators

H^{ij} matrix elements function of

$$t_{pq} \quad \overline{v}_{pqrs} \quad \overline{w}_{pqrstu} \quad U_{pk} \quad V_{pk}$$

Similarly for *A* and Ω

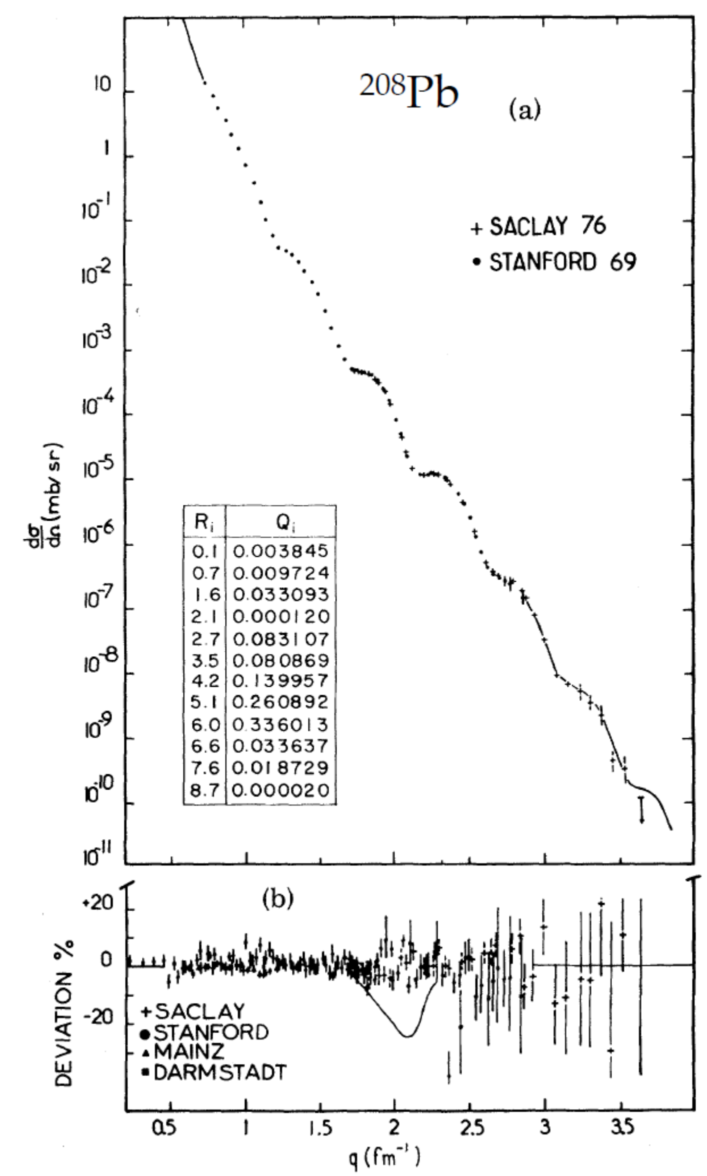
Six-index tensors
Too expensive to handle

NO2B approximation
1-3% error in closed shell
[Roth *et al.*, PRL 109 (2012) 052501]

PNO2B approximation
Particle-number conserving
[Ripoche, Tichai, Duguet, arXiv:1908.00765]

Electron scattering off nuclei

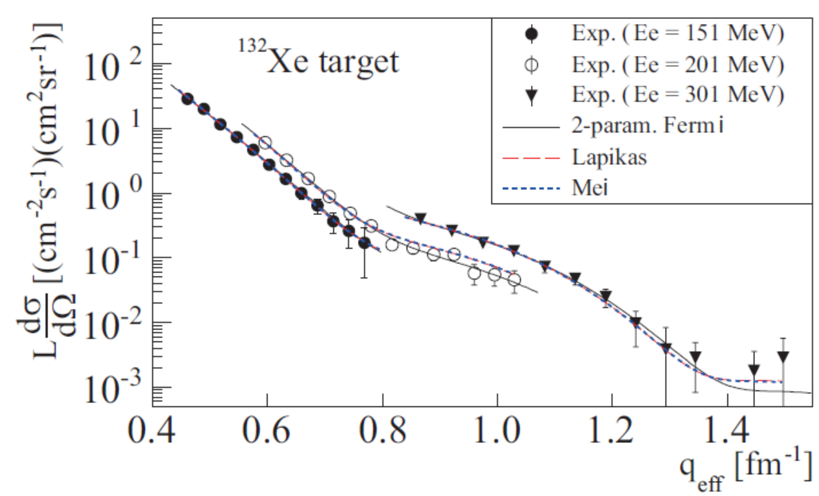
- ◉ Electrons constitute an optimal probe to study atomic nuclei
  - ○ Point-like → excellent spatial resolution
  - ○ EM weak and theoretically well constrained
- ◉ Accélérateur Linéaire @ Saclay (ALS)
  - ○ Electron accelerator (1969-1990)
  - ○ Refined data on tens of stable nuclei

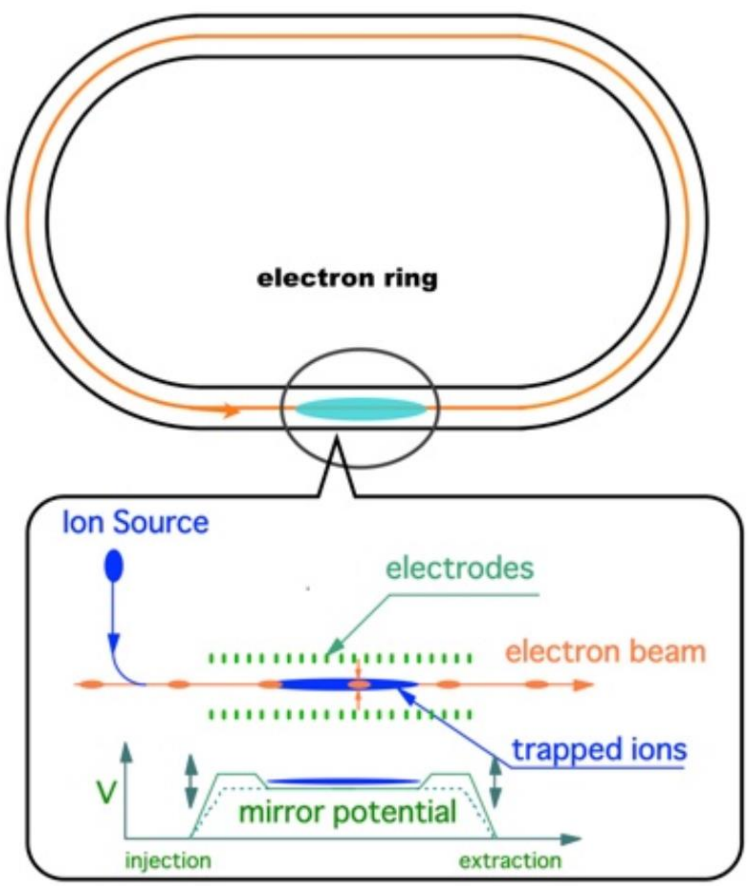


13 orders of magnitude!

[Frois *et al.* 1977]

[Tsukada *et al.* 2017]





➪ **Electron scattering off unstable nuclei?**
- ○ Challenge for the future
- ○ First physics experiments in 2017 with SCRIT @ RIKEN

Guidance for improved nuclear many-body Hamiltonians

Nuclear lattice calculations of 86 even-even nuclei up to A=48 and pure neutron matter *[Lu et al. 2018]*

¤ Leading-order pion-less EFT SU(4)-invariant with 2N and 3N interactions

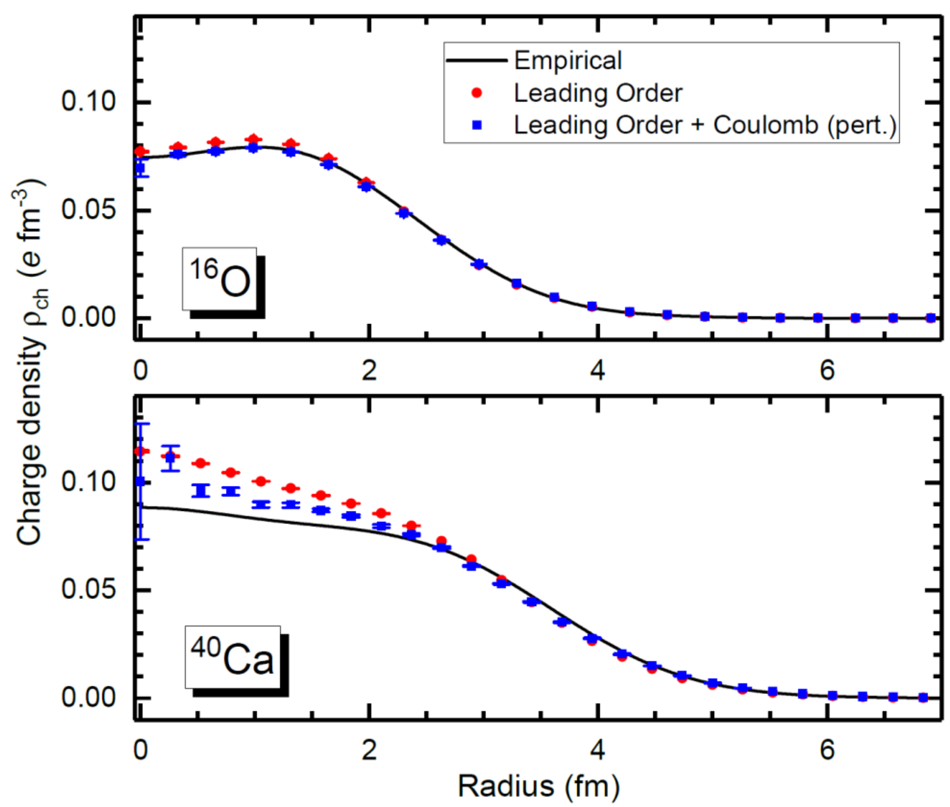
$C_2 \leftrightarrow$ 2N
$C_3 \leftrightarrow$ 3N
$S_L \leftrightarrow$ Local part
$S_{NL} \leftrightarrow$ Non-local part

Fit

Effective range r_0 averaged over $^1S_0$ and $^3S_1$
S-wave scattering length a_0 averaged over $^1S_0$ and $^3S_1$
$B(^3H)$
+ set of mid-mass nuclei

N=Z	B	Exp.	R_{ch}	Exp.	Cou.
^{3}H	8.48(2)	8.48	1.90(1)	1.76	0.0
^{3}He	7.75(2)	7.72	1.99(1)	1.97	0.73(1)
^{4}He	28.89(1)	28.3	1.72(1)	1.68	0.80(1)
^{16}O	121.9(1)	127.6	2.74(1)	2.70	13.9(1)
^{20}Ne	161.6(1)	160.6	2.95(1)	3.01	20.2(1)
^{24}Mg	193.5(2)	198.3	3.13(1)	3.06	28.0(1)
^{28}Si	235.8(4)	236.5	3.26(1)	3.12	37.1(2)
^{40}Ca	346.8(6)	342.1	3.42(1)	3.48	71.7(4)

Error < 4.5% on BE in ^{16}O and < 8.0% on R_c in ^{3}H



Coulomb effect beneficial

→ SU(4)-invariant LO very satisfactory for large A
→ Satisfatory pure neutron matter + volume/surface energy coefficients
→ Corrections from spin&isospin dependent terms

Novel many-body formalisms

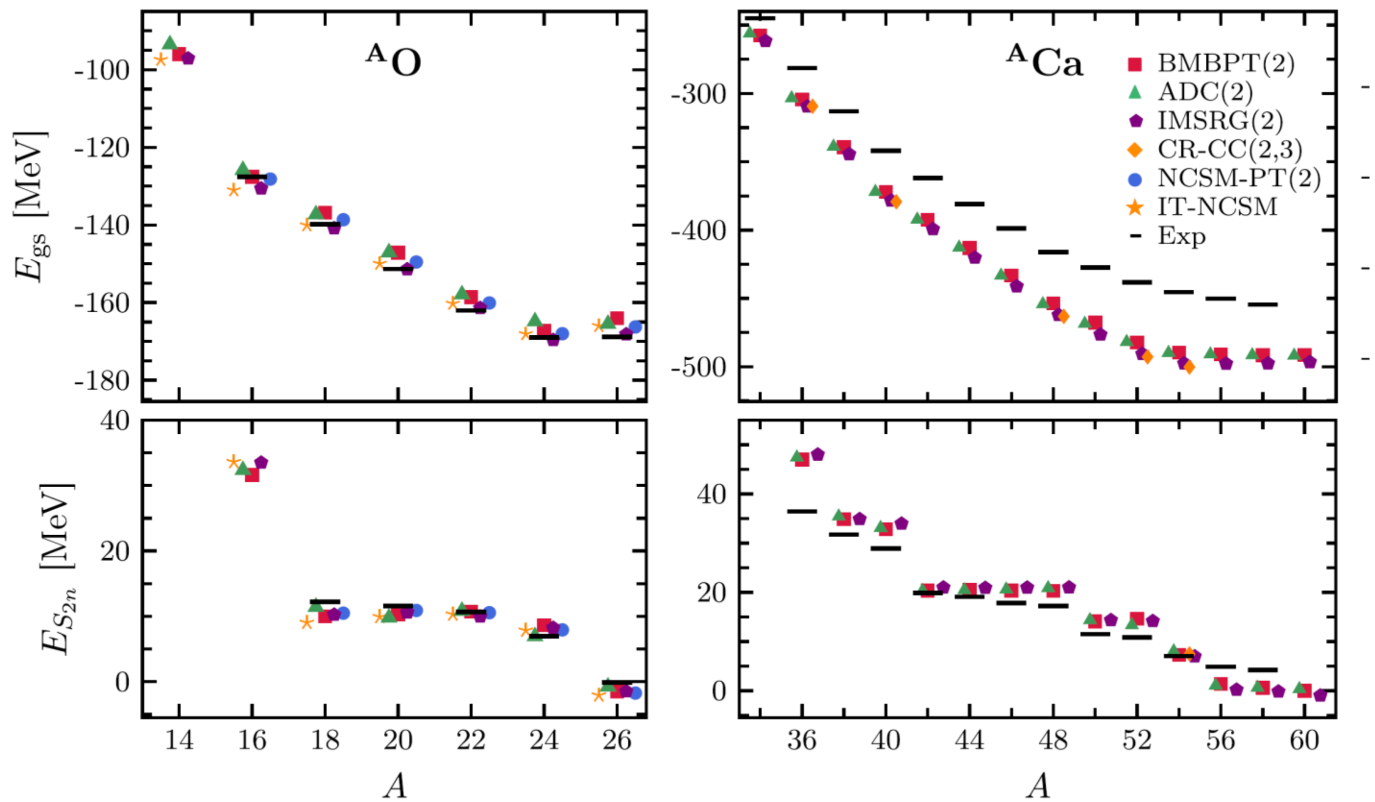
◉ No real free lunch but still look for best compromise
- ✓ Versatility (nuclei and/or states/observables)
- ✓ Accuracy
- ✓ CPU cost

[Duguet, Signoracci 2016]

◉ Optimal many-body method for open-shell nuclei: **Bogoliubov many-body perturbation theory**

→ Code for automated generation of many-body diagrams *[Arthuis et al. 2018]*

[Tichai et al. 2018]



Calculation details

Chiral NN+3N Hamiltonian
SRG α = 0.08 fm^4
13 major shells (1820 s.p. states)
Canonical HFB reference

Runtime

NCSM:	20.000 hours
MCPT:	2.000 hours
IMSRG(2):	1.500 hours
SCGF(2):	400 hours
BMBPT:	**< 1min !**

→ 2-3% agreement of all methods with exact results (IT-NCSM)
→ Different truncation schemes yield consistent description of open-shell nuclei
→ BMBPT optimal to systematically test next generation of Chiral EFT nuclear Hamiltonians