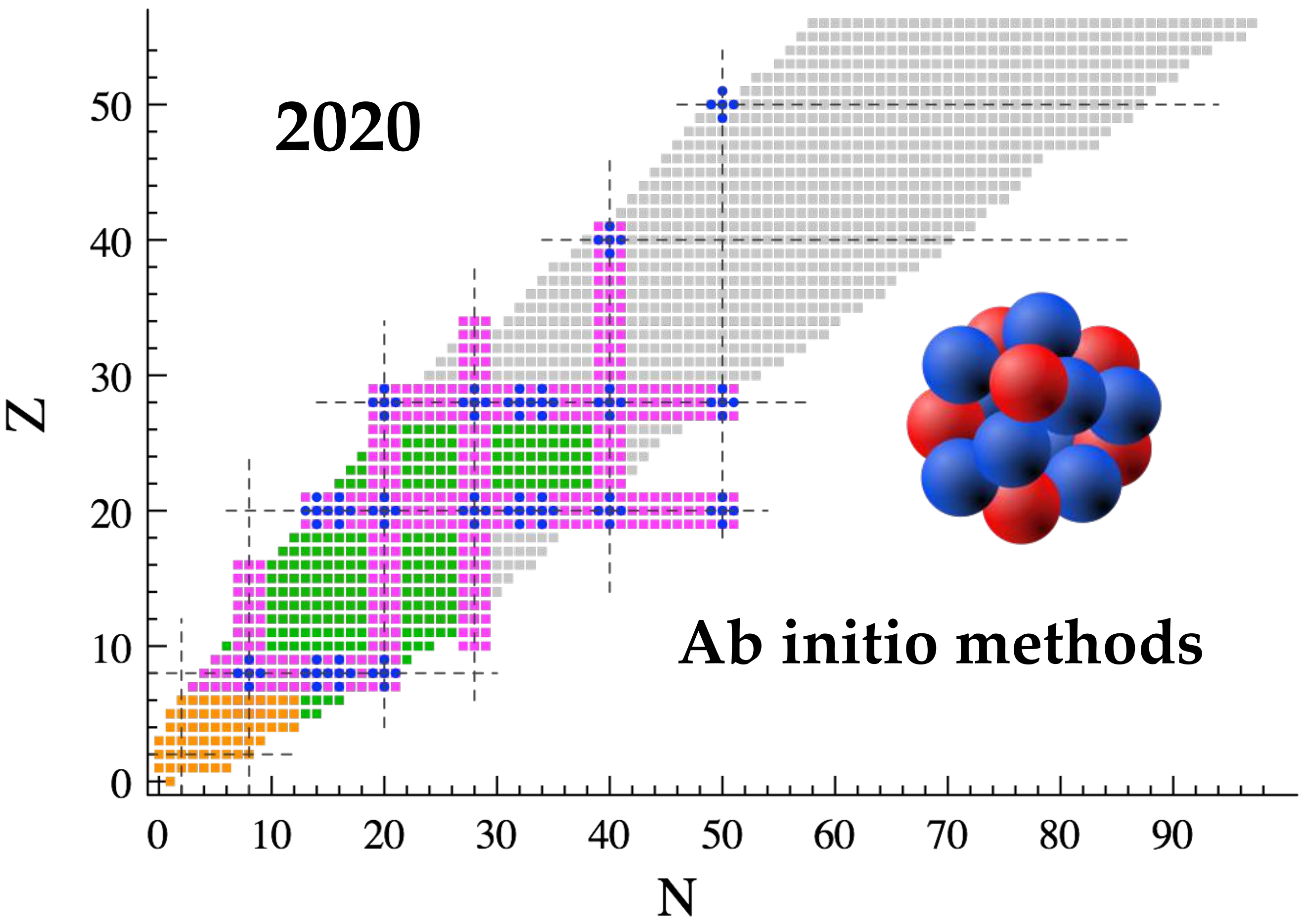
Problème quantique à N-corps en physique nucléaire

A journey through a general introduction and an overview of the « ab initio » approach



Thomas DUGUET

DPhN, CEA-Saclay, France
IKS, KU Leuven, Belgium

1ère réunion générale du GDR NBODY, 8-10 janvier 2020, Lille

Contents

- Introduction to low-energy nuclear physics
  - Phenomenology
  - Rationale from the theoretical viewpoint
- Strong inter-nucleon forces
  - Phenomenology and modern modelling
- The ab initio nuclear many-body problem
  - Specificities
  - Recent developments
  - Status of ab initio calculations of medium-mass atomic nuclei
- Conclusions and perspectives

Contents

- Introduction to low-energy nuclear physics
  - Phenomenology
  - Rationale from the theoretical viewpoint
- Strong inter-nucleon forces
  - Phenomenology and modern modelling
- The ab initio nuclear many-body problem
  - Specificities
  - Recent developments
  - Status of ab initio calculations of medium-mass atomic nuclei
- Conclusions and perspectives

Elementary facts and « big » questions about nuclei

○ 252 **stable** isotopes, ~3100 synthesized in the lab

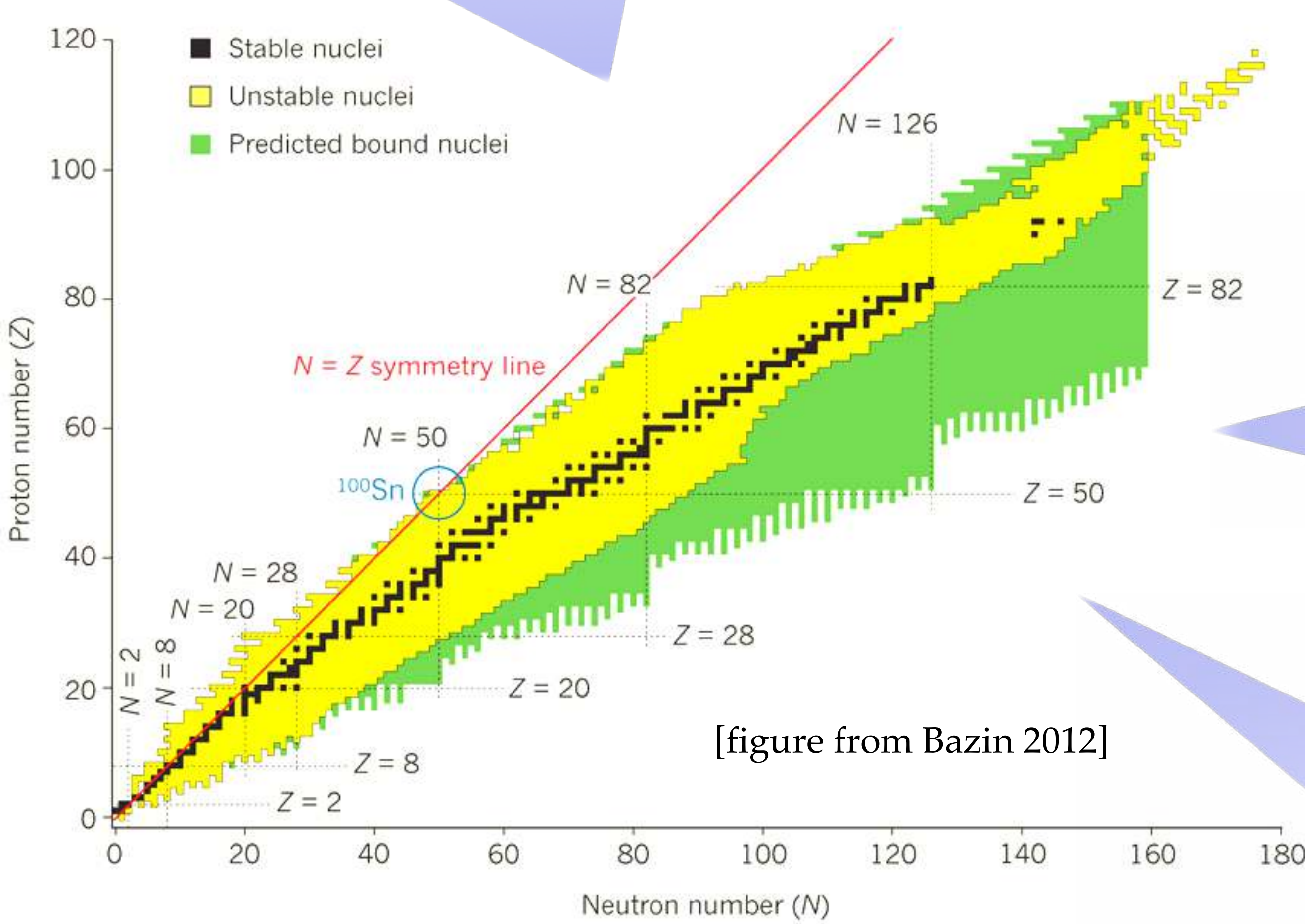
○ **How many** bound (w.r.t strong force) nuclei exist; 9000?

Oganesson $_{118}$Og added to Mendeleïev table in 2016

○ **Heaviest** synthesized element Z=118

○ **Heaviest possible** element?

○ Enhanced stability near Z=120?126?



[figure from Bazin 2012]

2p decay beyond the proton drip line in ^{45}Fe in 2002

○ Modes of **instability** (α, p, β, γ decays, fission)

○ Are there more exotic/rare decay modes?

Ex: ν-less 2β decay = test of standard model?

Gravitational wave + kilonova from neutron stars merger in 2017

○ Elements **up to Fe** produced in stellar fusion

○ How have heavier elements been produced?

○ Exotic r-process nucleosynthesis ; but where?

Updated in 2019 to Z=9 (22 neutrons) and Z=10 (24 neutrons)

○ Neutron **drip-line** known up to ~~Z=8 (16 neutrons~~)

○ Where is the neutron drip-line beyond Z=10?

Shown to disappear away from stability in 1975/1993

○ Over-stable "magic" nuclei (2, 8, ~~20, 28,~~ 50, 82, …)

○ How **other magic numbers** evolve with N-Z?

The atomic nucleus as a 4-components quantum mesoscopic system
An extremely rich and diverse phenomenology

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

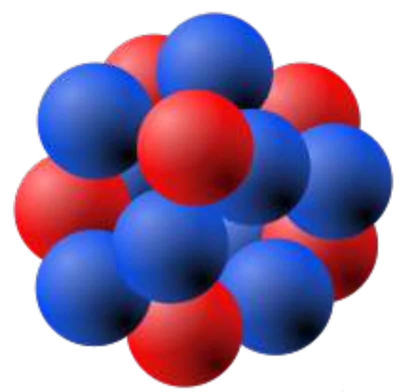
Several scales at play:

p & n momenta ~ $\mathbf{10^8}$ eV

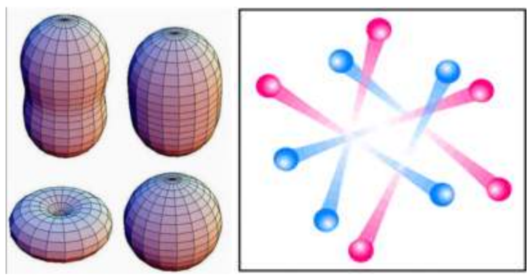
Separation energies ~ $\mathbf{10^7}$ eV

Vibrational excitations~ $\mathbf{10^6}$ eV

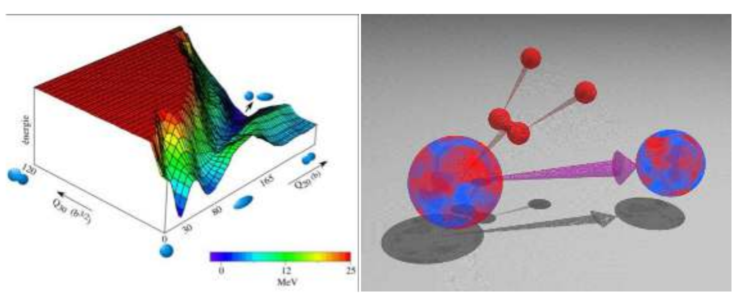
Rotational excitations ~ $\mathbf{10^4}$ eV



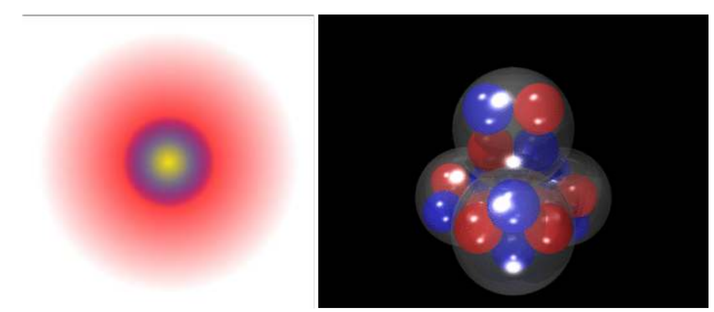
Ground state
Mass, size, superfluidity, e.m. moments…



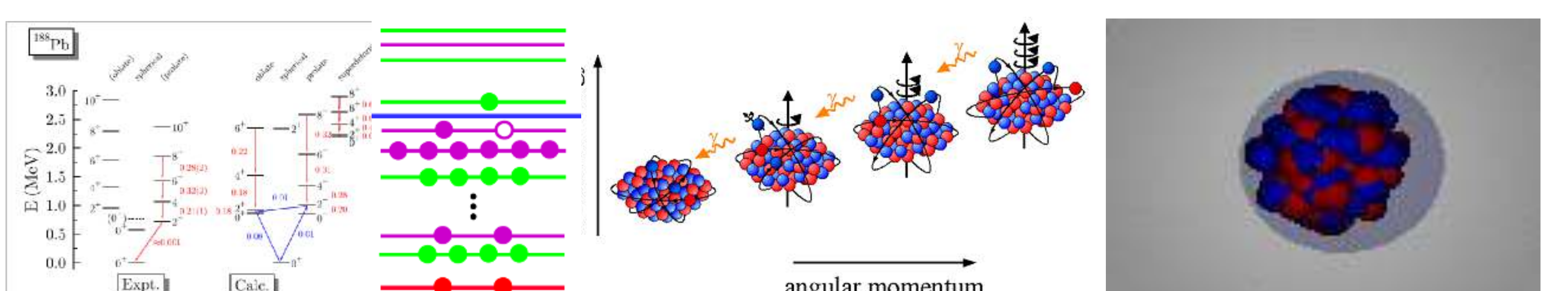
Radioactive decays
β, 2β, 0ν2β, α, p, 2p, (≠)fission, …



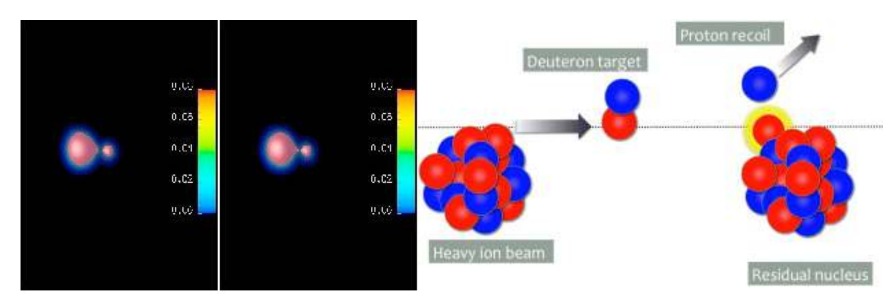
Exotic structures
Clusters, halos, …



Spectroscopy
Excitation modes



Reaction processes
Fusion, transfer, knockout, …



The atomic nucleus as a laboratory test
A multi-scale and multi-physics connector

Nuclei and homogeneous nuclear matter

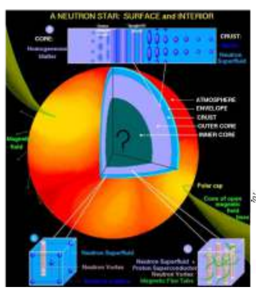
Many scales at play, e.g.

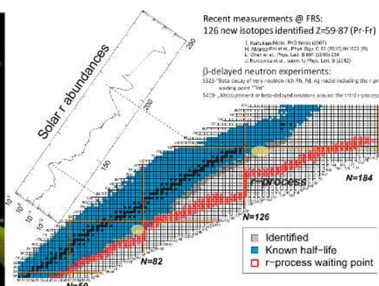
Nuclei: 10^{-15} m

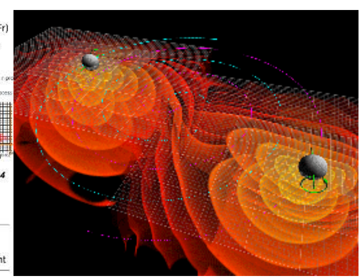
Factor 10^{19}!

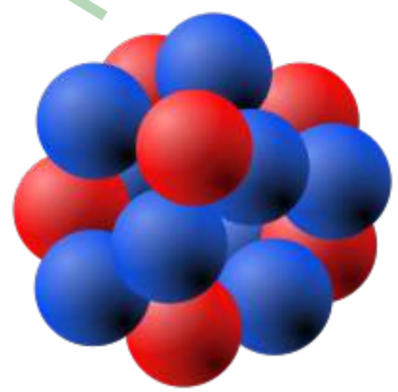
Neutron star: 10 km

Astrophysics
Neutron star, supernovae, nucleo-synthesis (GW and kilonova)…

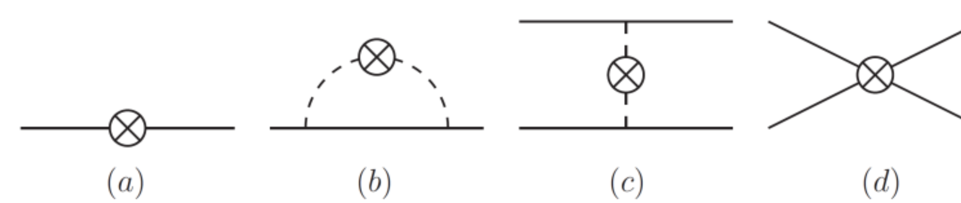




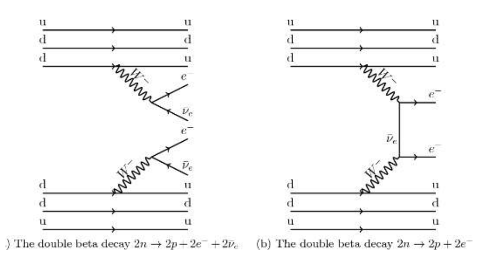




Dark matter
Nucleus-WIMP scattering

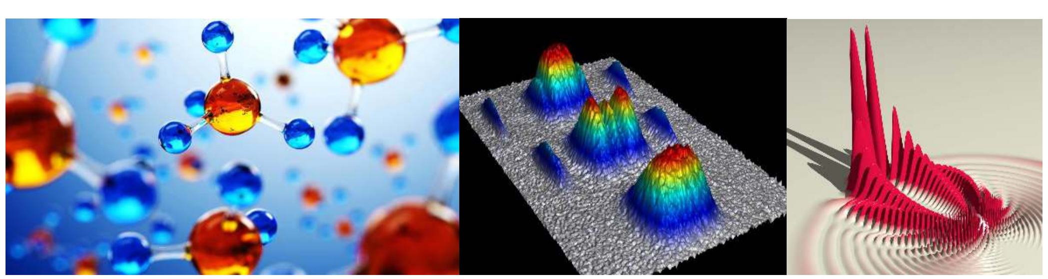


Standard model of particle physics
0ν2β, unitarity of CKM matrix, PT



$$\begin{bmatrix} d' \\ s' \\ b' \end{bmatrix} = \begin{bmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{bmatrix} \begin{bmatrix} d \\ s \\ b \end{bmatrix}.$$

Mesoscopic many-body systems
Molecules, atoms, cold atom gases…



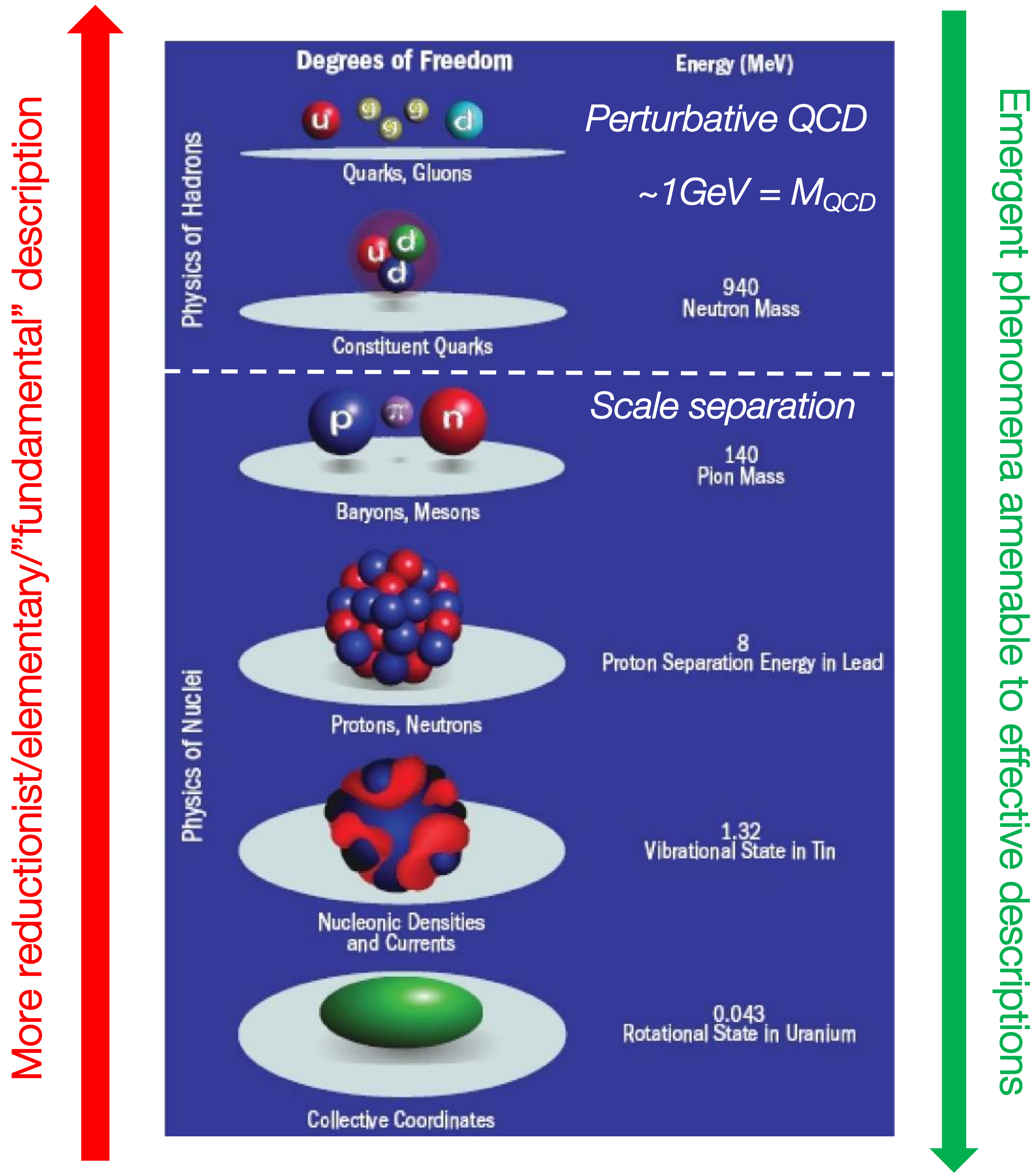
Large-scale experiments
Radioactive ion beam facilities

FACILITY FOR RARE ISOTOPE BEAMS
GANIL spiral2
ISOLDE
RIBF
RIKEN NISHINA CENTER
RIKEN Nishina Center for Accelerator-Based Science
Introduction to RI Beam Factory and Users' Information
FAIR
Facility for Antiproton and Ion Research in Europe GmbH

Contents

- Introduction to low-energy nuclear physics
    - Phenomenology
    - Rationale from the theoretical viewpoint
- Strong inter-nucleon forces
    - Phenomenology and modern modelling
- The ab initio nuclear many-body problem
    - Specificities
    - Recent developments
    - Status of ab initio calculations of medium-mass atomic nuclei
- Conclusions and perspectives

Energy scales and degrees of freedom



High-energy nuclear, i.e. hadronic, physics

- Realm of Quantum Chromo Dynamics
- Quarks and gluons
- Chiral symmetry of QCD
- Confinement and asymptotic freedom

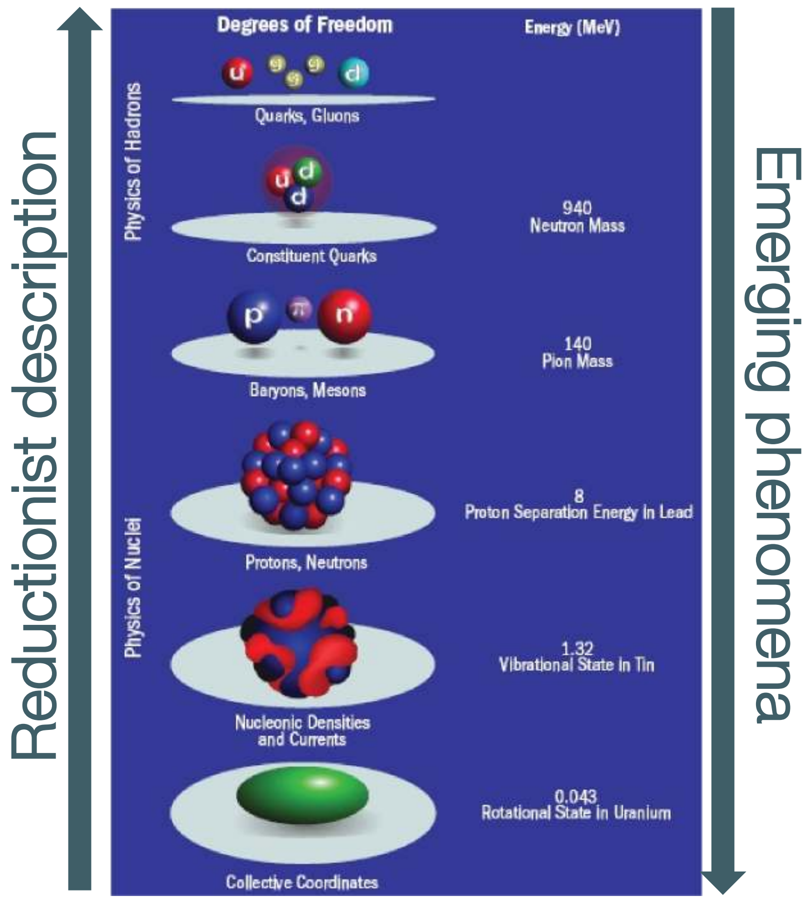
The description

- Depends on the energy scale
- Must rely on appropriate choice of DOFs
- Must encode the key symmetries

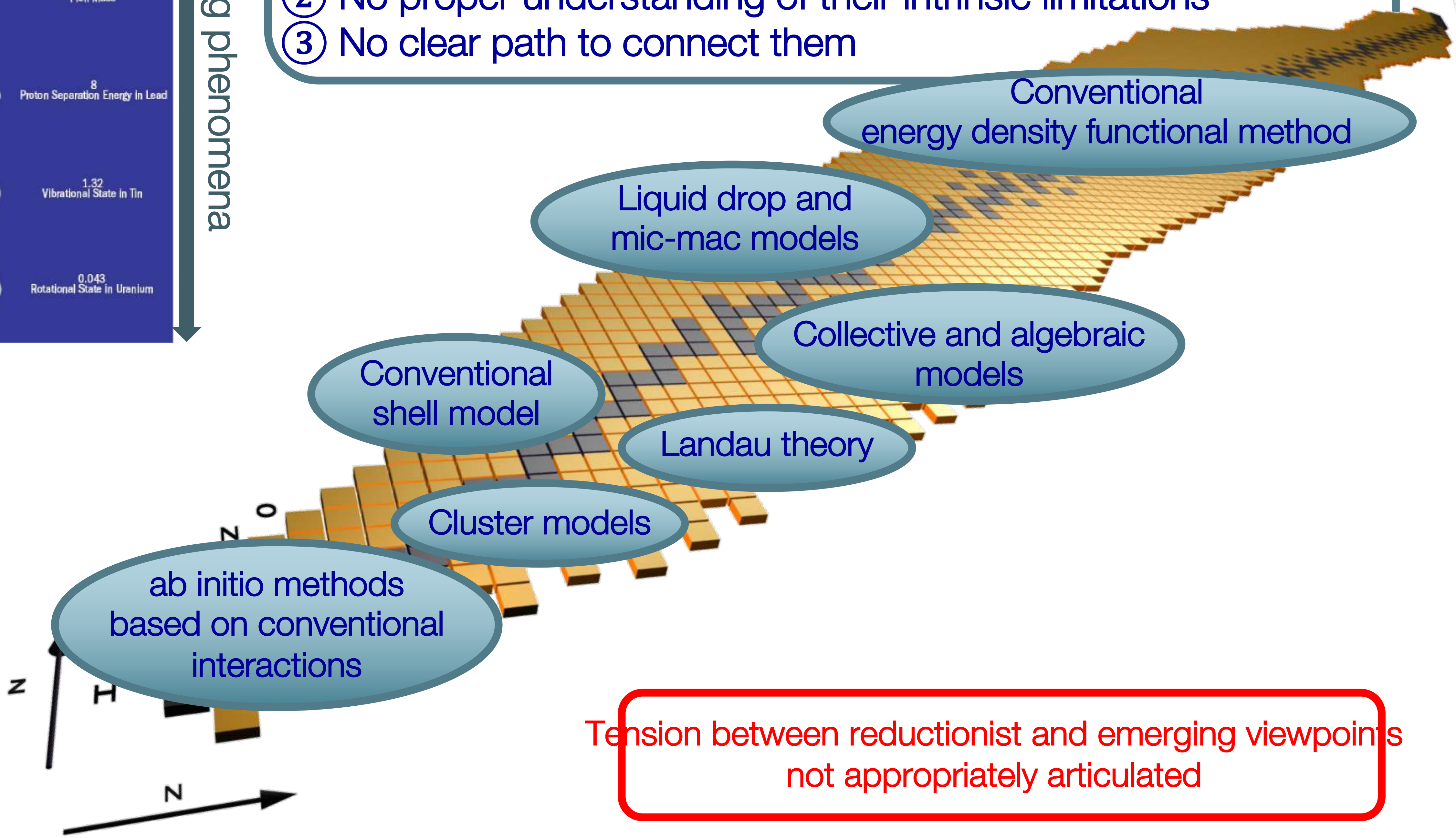
Low-energy nuclear physics

- Of order of ~150MeV (M_{nuc}, m_{π}…)
- Nucleons and pions
- Chiral symmetry (breaking) of QCD
- Even more effective DOFs for MeV scale

Nuclear physics moving from a plurality of nuclear models…

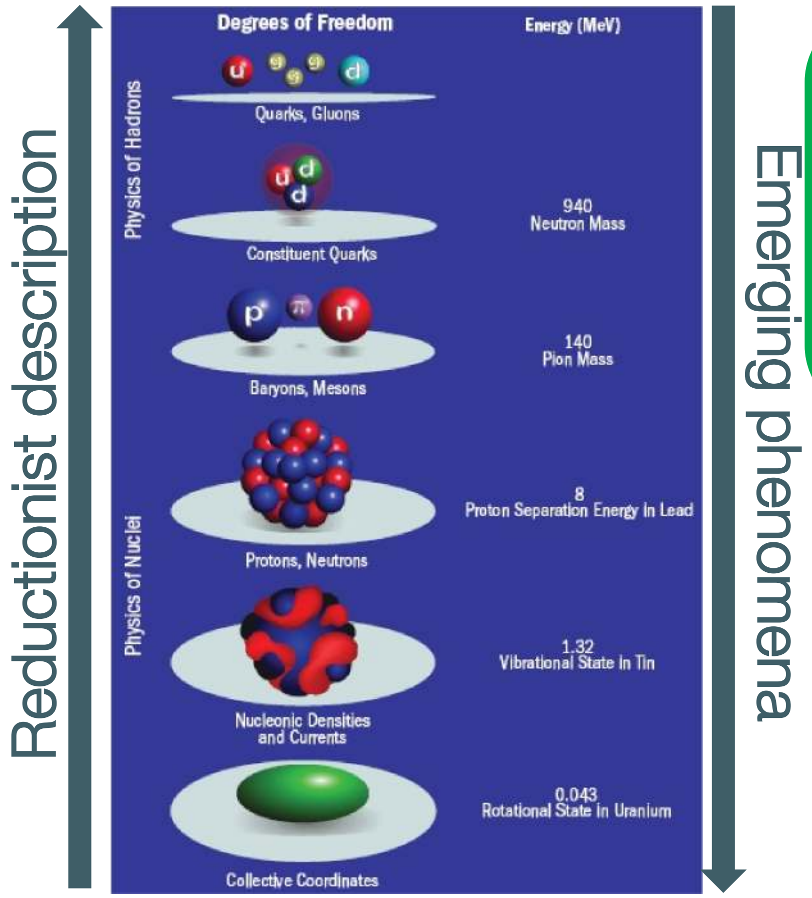


→ Useful to identify relevant d.o.f and symmetries
→ Decent account of phenomena based on employed d.o.f
BUT
① No systematic improvement towards accuracy
② No proper understanding of their intrinsic limitations
③ No clear path to connect them



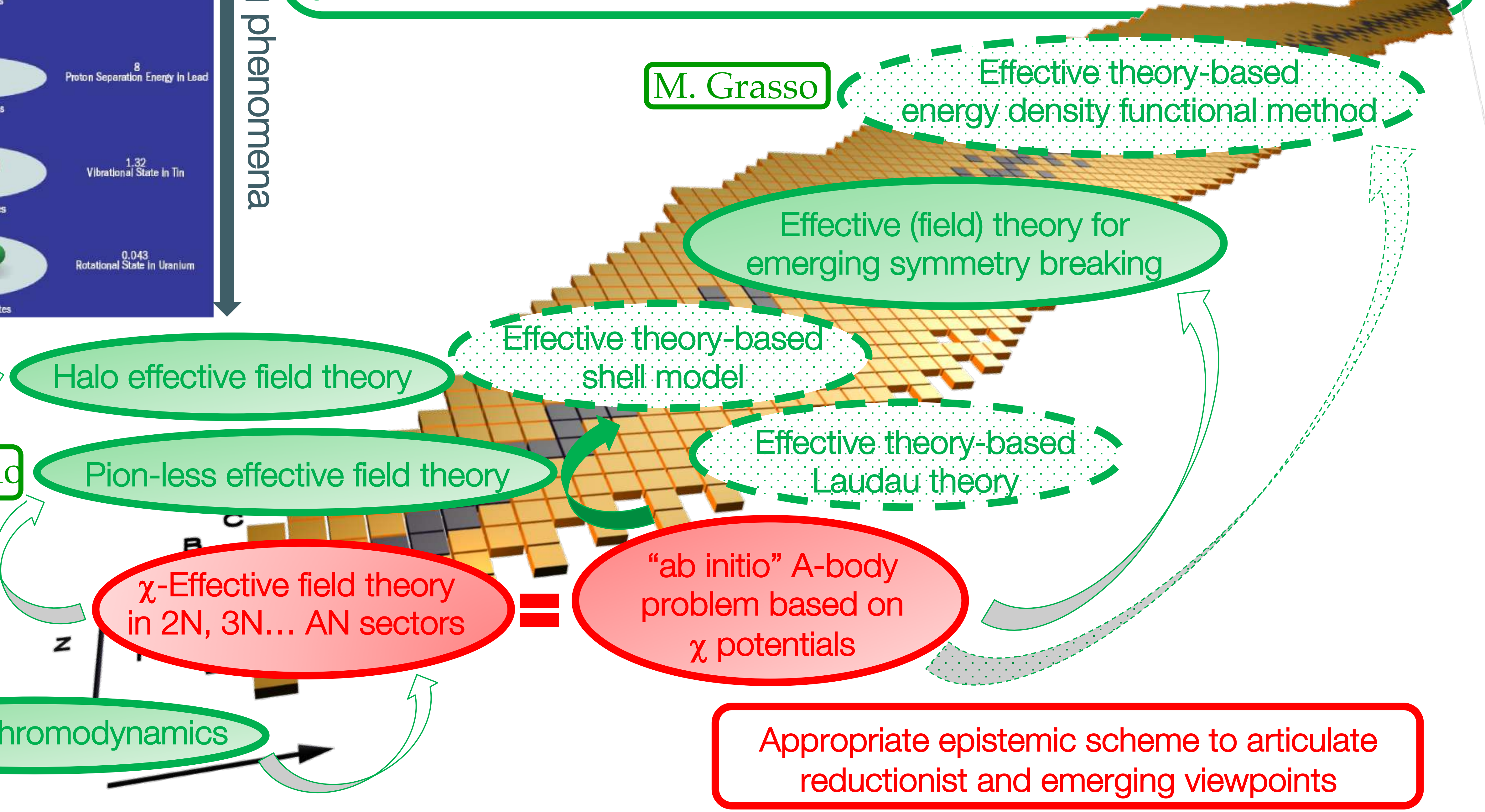
Tension between reductionist and emerging viewpoints not appropriately articulated

…to an arborescence of nuclear effective (field) theories



Rationale of effective theories

1. Identify appropriate energy scales / d.o.f / symmetries
2. All interactions complying with symmetries are compulsory
3. Naturalness provides power counting (+ possible fine tuning)
4. Fix LECs from data or from underlying effective theory



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

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

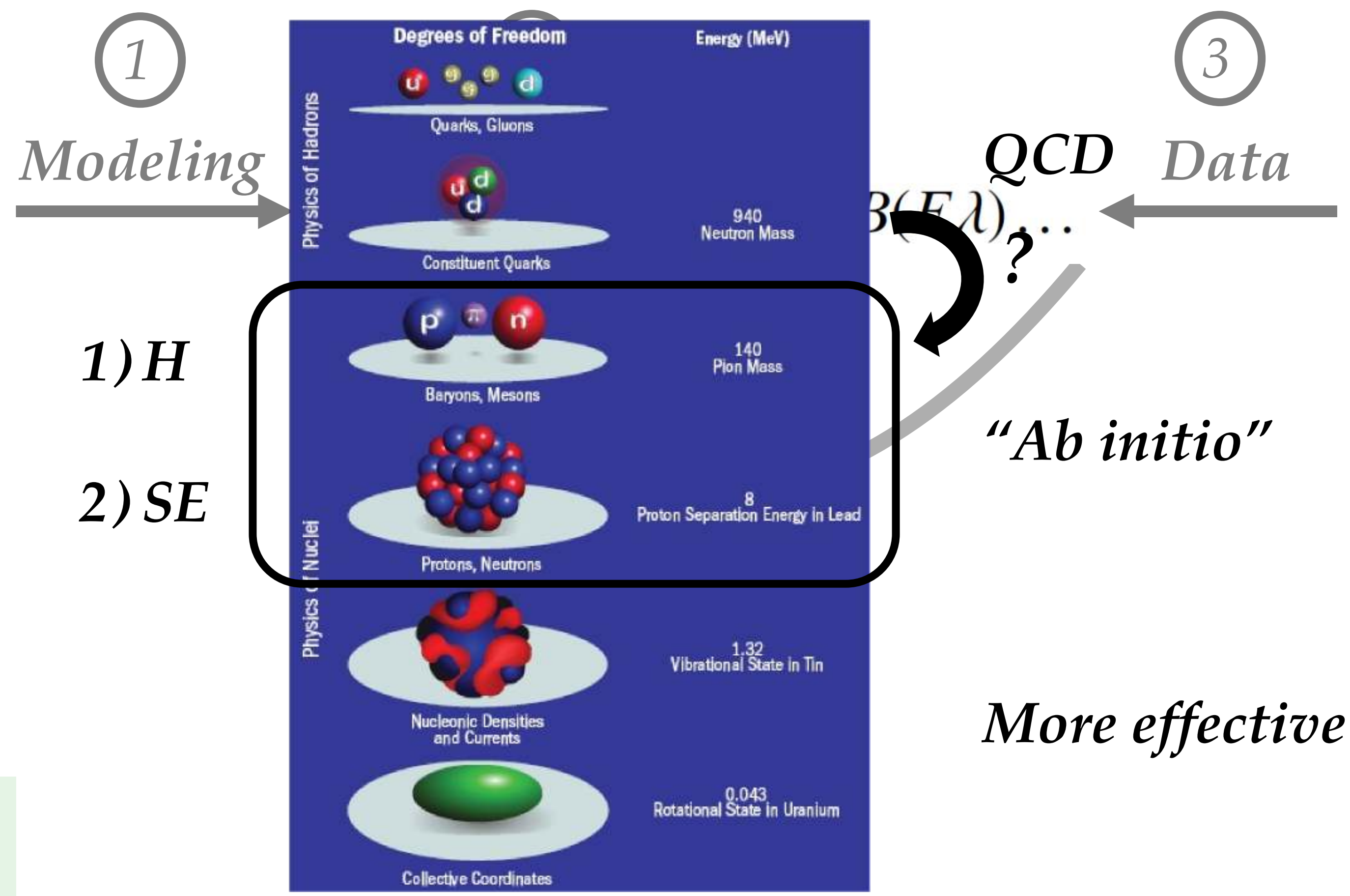
$$H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$$

A-body Hamiltonian

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

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) ***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?
Consistent construction of other operators?

Contents

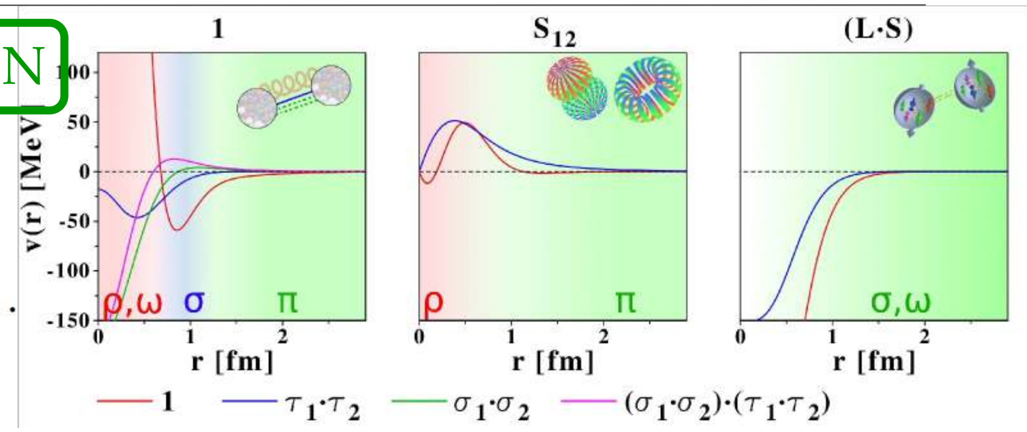
- ◉ Introduction to low-energy nuclear physics
  - ○ Phenomenology
  - ○ Rationale from the theoretical viewpoint
- ◉ Strong inter-nucleon forces
  - ○ Phenomenology and modern modelling
- ◉ The ab initio nuclear many-body problem
  - ○ Specificities
  - ○ Recent developments
  - ○ Status of ab initio calculations of medium-mass atomic nuclei
- ◉ Conclusions and perspectives

Phenomenology of inter-nucleon interactions

$$H \equiv \sum_{i=1}^{A} \frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2}\sum_{i\neq j}^{A} V^{2N}(i,j) + \frac{1}{6}\sum_{i\neq j\neq k}^{A} V^{3N}(i,j,k) + \ldots$$

$$= \sum_{\alpha\beta} t_{\alpha\beta} a^{\dagger}_{\alpha} a_{\beta} + \left(\frac{1}{2!}\right)^2 \sum_{\alpha\beta\gamma\delta} \bar{v}^{2N}_{\alpha\beta\gamma\delta} a^{\dagger}_{\alpha} a^{\dagger}_{\beta} a_{\delta} a_{\gamma} + \left(\frac{1}{3!}\right)^2 \sum_{\alpha\beta\gamma\delta\zeta\epsilon} \bar{v}^{3N}_{\alpha\beta\gamma\delta\zeta\epsilon} a^{\dagger}_{\alpha} a^{\dagger}_{\beta} a^{\dagger}_{\gamma} a_{\epsilon} a_{\zeta} a_{\delta} + \cdots$$

2N



Old view = meson exchanges

1. Interactions between effective point-like four-components fermions

   a. Nucleon = neutron/proton (±½ isospin projections) with spin up/down (±½ spin projections)

2. Complex operator structure in space*spin*isospin spaces

   a. **Strong central + spin-orbit + tensor operators**

   b. Dominant two-nucleon and sub-leading (but mandatory) three-nucleon operators

3. Infra-red source of non-perturbativeness

   a. **Large scattering lengthes** (near unitarity) in s-wave channels = nn virtual state/np bound state

S=0 T=1   S=1 T=0

4. Ultra-violet source of non-perturbativeness

   c. **Short-range repulsion**

Modern constructive approach = effective field theory

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

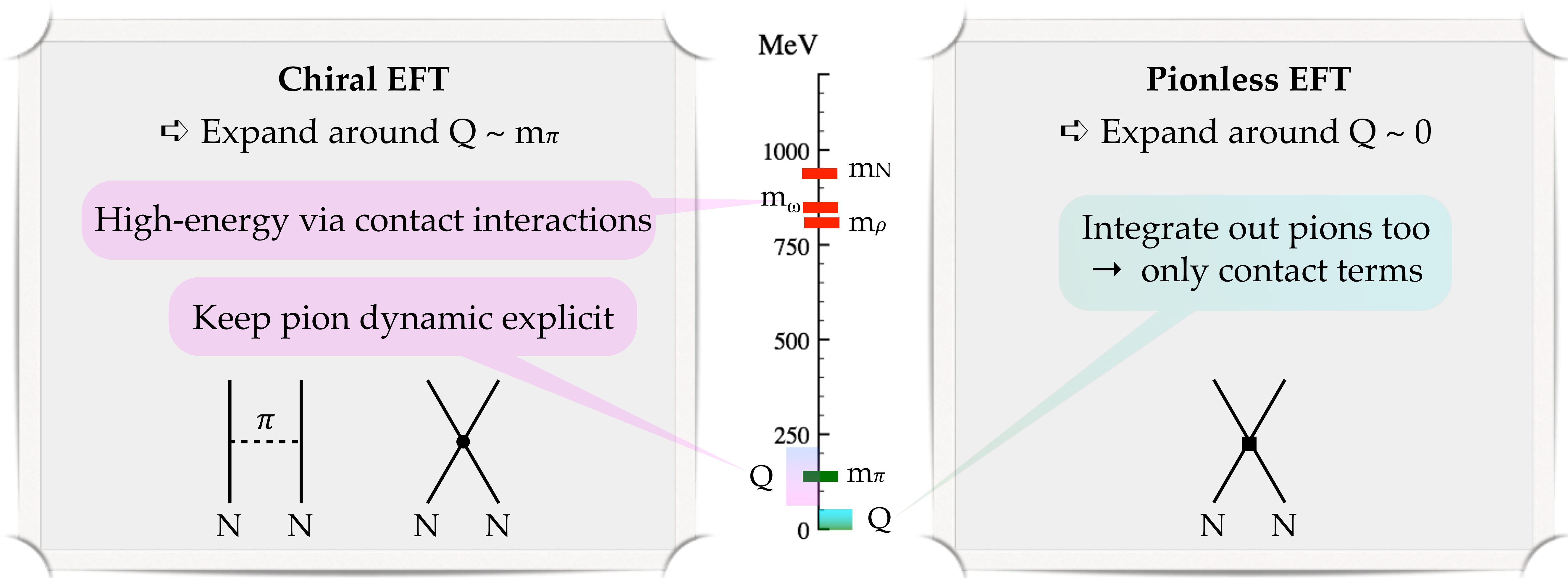
Typical momentum at play ← Q/Λ → High energy scale (physics beyond not included explicitly)

2. Parametrize physics beyond Λ + write #∞ terms allowed by **(broken) symmetries of underlying 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 effective field theory = Weinberg power counting

1) Interaction diagrams are made out of a) nucleon | and pion - - - propagators
b) pion-nucleon and (derivative) k-nucleon contact vertices

Goal of PC: estimate the power ν of the law $(Q/\Lambda_\chi)^\nu$ ith which each diagram scales

2) Naive Dimensional Analysis
a) nucleon propagator carries Q^{-1}
b) pion propagator carries Q^{-2}
b) derivative operator carries Q
c) loop integration brings Q^4

$$\frac{1}{m_\omega^2 + Q^2} \approx \frac{1}{m_\omega^2}\left(1 - \frac{Q^2}{m_\omega^2} + \frac{Q^4}{m_\omega^4} - + \ldots\right)$$

Fits with PC in powers of $Q/m_\omega \approx Q/\Lambda_\chi$

Connected diagrams

$$\nu = 2k - 4 + 2L + \sum_i \Delta_i$$

with $\Delta_i \equiv d_i + \frac{n_i}{2} - 2$

k = k-nucleon sector
L = # of loops
d_i = # of derivatives/pion masses at vertex i
n_i = # of nucleon fields at vertex i

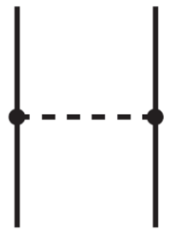
Hierarchy of k-body forces: 3N (4N) starts 2 (4) orders after 2N

$\Delta_i \geq 0$
$\nu \geq 0$

Chiral symmetry
Finite # at given order

Weinberg PC for interaction potential → **Insert into dynamical, i.e. A-body Schroedinger, equation to access observables**

3) Examples: diagrams in 2-nucleon sector at Leading Order (LO) with ~Q^0 ($\nu = 0$ from k=2, L=0, Δ_i=0)



$$V_{1\pi}^{(0)}(\boldsymbol{p}', \boldsymbol{p}) = -\frac{g_A^2}{4f_\pi^2}\, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \frac{\boldsymbol{\sigma}_1 \cdot \boldsymbol{q}\, \boldsymbol{\sigma}_2 \cdot \boldsymbol{q}}{q^2 + m_\pi^2}$$

Tensor operator

1π exchange (1PE)

$$V_{\rm ct}^{(0)}(\boldsymbol{p}', \boldsymbol{p}) = C_S + C_T\, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

Central operator (no q dependence)

Pure contact term (CT)

4) **Consistent construction of other operators (e.g. coupling to electroweak or WIMP probes)**

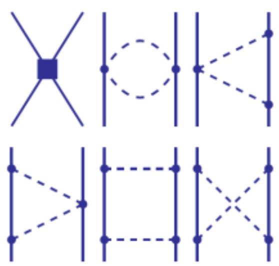
Chiral effective field theory = interactions expansion

2N Force | 3N Force | 4N Force

LO $(Q/\Lambda_\chi)^0$

2N tree level CT (key for large a_s)
2N tree-level 1PE (key for deuteron)

NLO $(Q/\Lambda_\chi)^2$

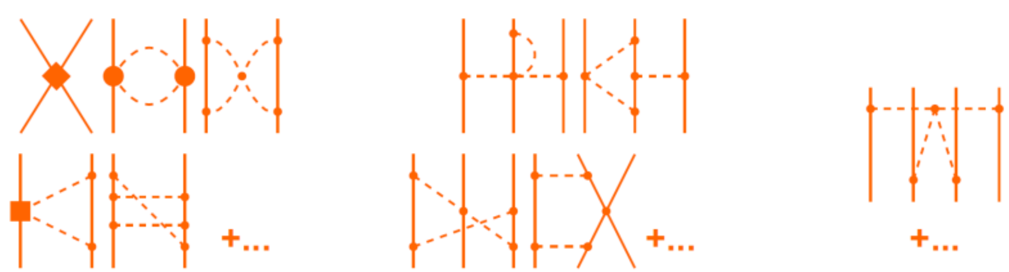


2N tree level CT (spin-orbit, tensor)
2N one-loop 2PE (weak)

NNLO $(Q/\Lambda_\chi)^3$

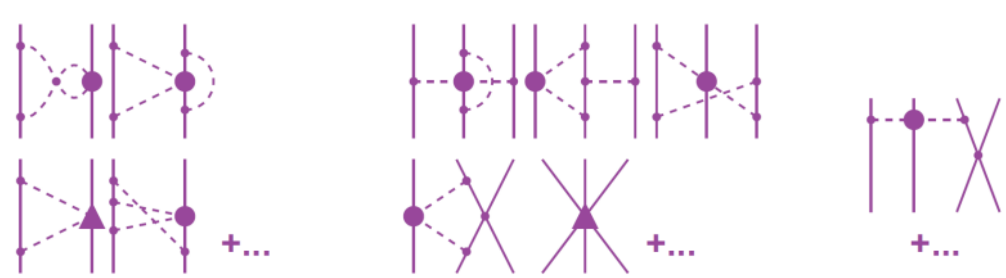
2N one-loop 2PE (brings intermediate range attraction; no new param)
3N tree-level 2PE, 1PE-CT, CT (key for saturation, 3N scattering, drip lines…)

N^3LO $(Q/\Lambda_\chi)^4$



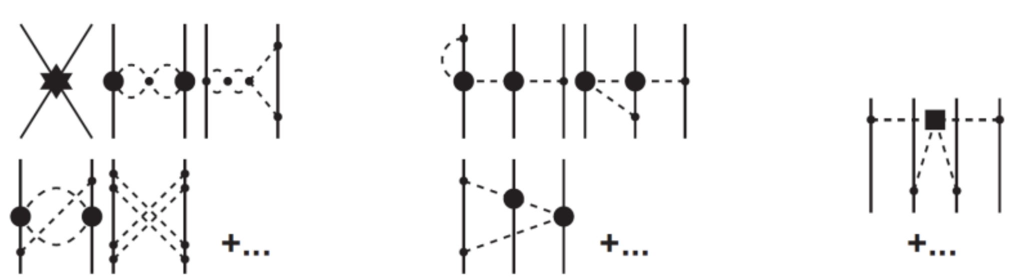
2N tree-level CT, one-loop 2PE, two-loop 2PE, 3PE
3N one-loop 3PE, 2PE-CT… (no new param)
4N… (weak; no new param)

N^4LO $(Q/\Lambda_\chi)^5$



2N two-loop 2PE, 3PE
3N… (derived but little used; large + solve the n-d A_y puzzle)
4N… (not yet derived)

N^5LO $(Q/\Lambda_\chi)^6$



1) **Finite number of terms up to given ν**
2) No ν = 1 due to parity/time reversal
3) 3N force cancels at ν = 2
4) **Proliferation = need fast convergence**
5) 3N at N^2LO and 4N at N^3LO
6) **Consistency between k-body sectors**
7) **LECs of contacts fitted to few-body data**
8) Estimate of error from $(Q/\Lambda_\chi)^{\nu+1}$

Major challenges

1) Can k-body, k>3, be omitted in A>>3?
2) Order by order renormalization? New PC?
3) $N^{3/4}LO$ 2N for high precision; 3N? 4N?

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

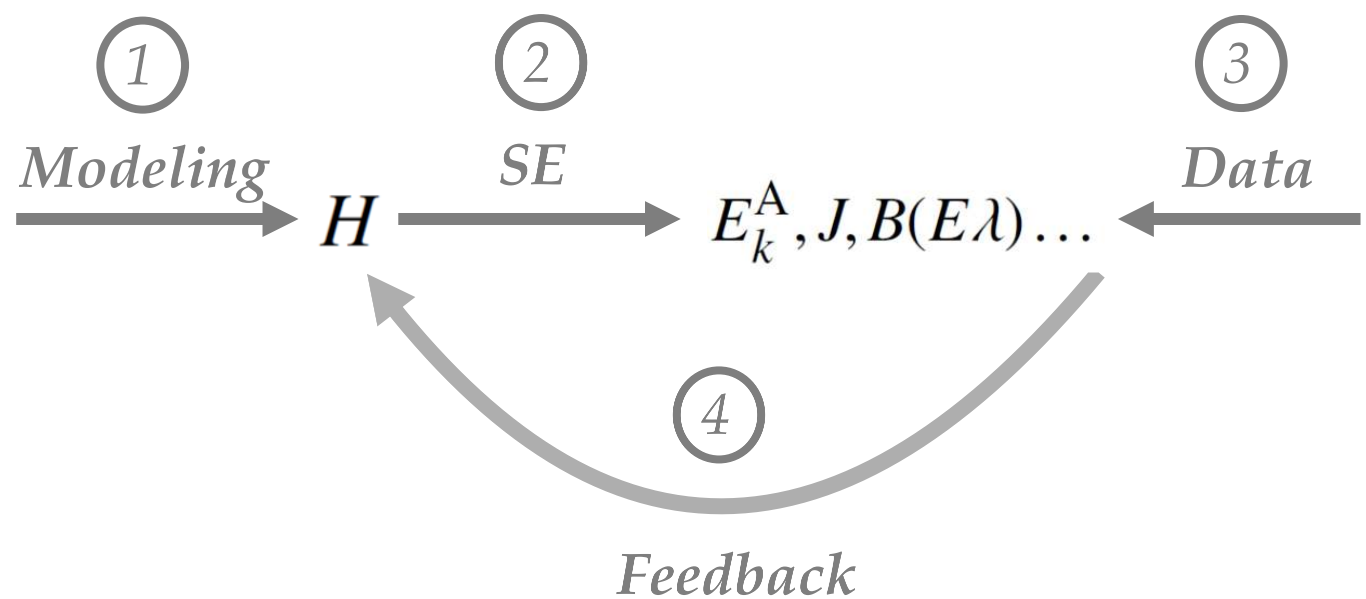
$$H = T + V^{2N} + V^{3N} + V^{4N} + \ldots + V^{AN}$$

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 *Hamiltonian&operators*

Explicit form of V^{2N}, V^{3N} can be built
Chiral EFT offers sound connection to QCD
Many-body forces as a result of effective d.o.f
Consistent construction of other operators

② *Schroedinger equation*

Can we solve the SE with relevant 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?

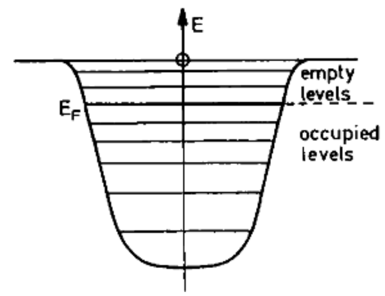
Contents

- Introduction to low-energy nuclear physics
  - Phenomenology
  - Rationale from the theoretical viewpoint
- Strong inter-nucleon forces
  - Phenomenology and modern modelling
- The ab initio nuclear many-body problem
  - Specificities
  - Recent developments
  - Status of ab initio calculations of medium-mass atomic nuclei
- Conclusions and perspectives

Specificities of atomic nuclei: mean field

1) **Self-bound system**
2) **Neutrons & protons**
3) **SU(2) sym. + strong L.S**

Mean-field approximation

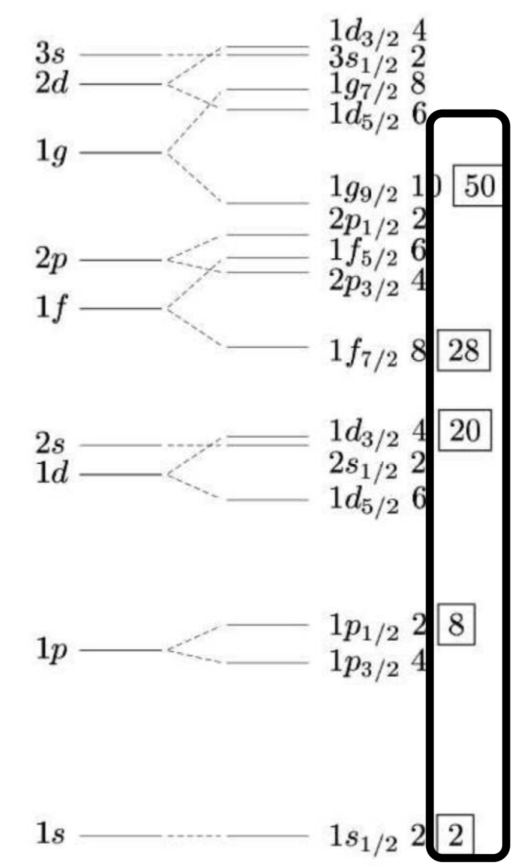


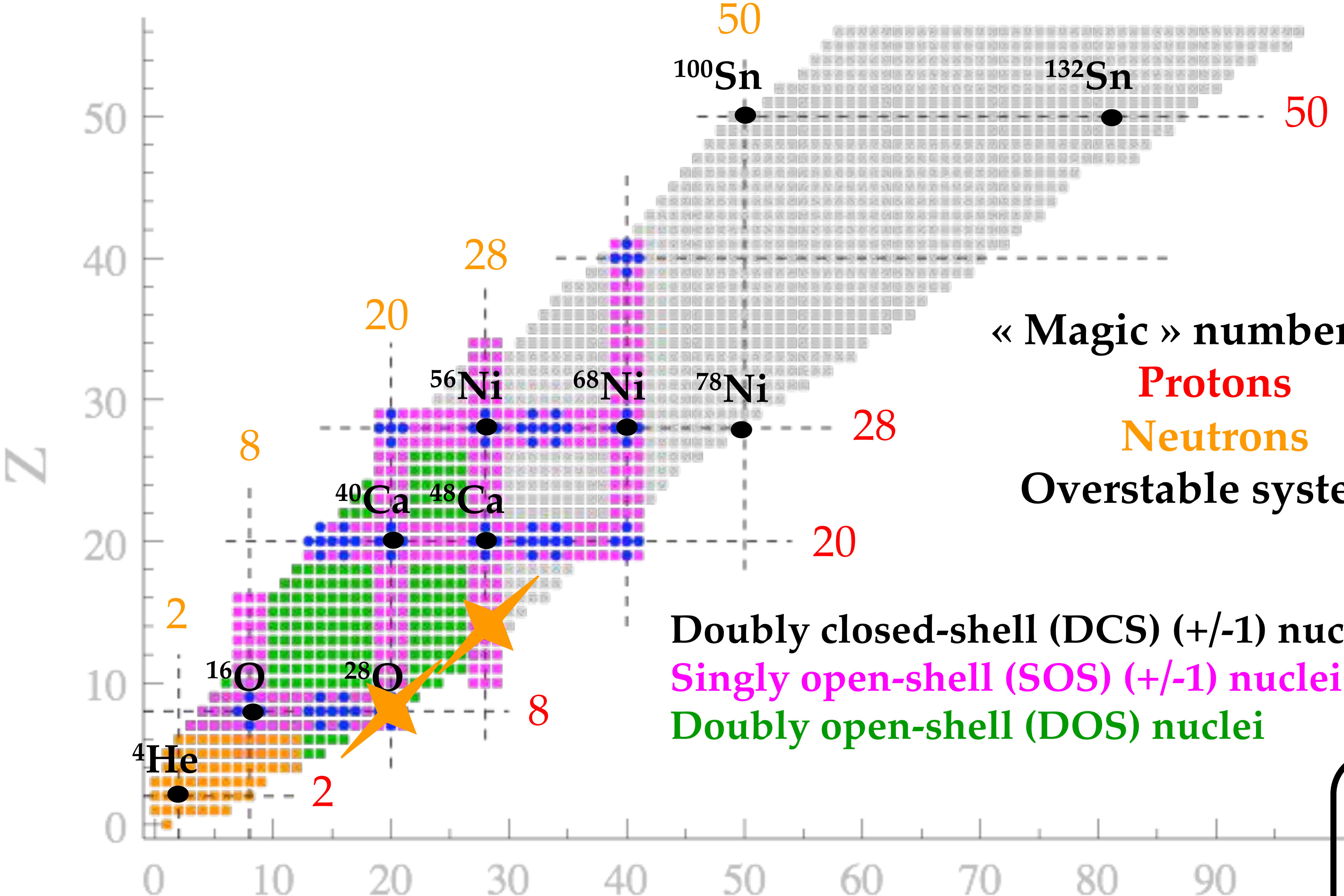
Average potential

Specificities

1) **Self created/centered**
2) **One for each species**
3) **j=l+s → 2j+1 degeneracy**

Filling of nuclear shells





Disappearance of N=20, 28 magicity away from stability

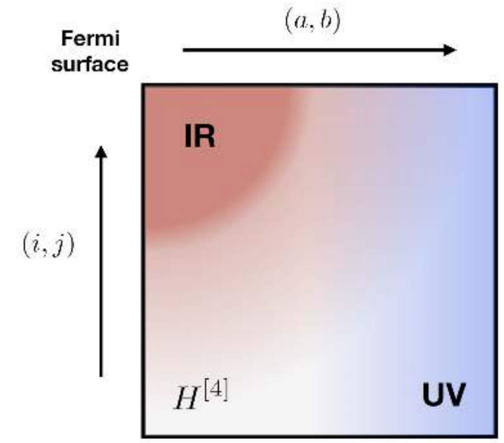
Mostly *open-shell* ground-states

Strong (« static ») correlations

Specificities of atomic nuclei: many-body correlations

1) Short-r repulsion
2) Bound np/Virtual nn
  2a) Large nn/pp a_s
  2b) Strong np tensor

Beyond mean-field expansion



Residual interaction

Many-body correlations

1) Dynamic corr. in UV
2) Strong static corr. in IR
  2a) Pairing in SOS
  2b) Collect. Quad. in DOS

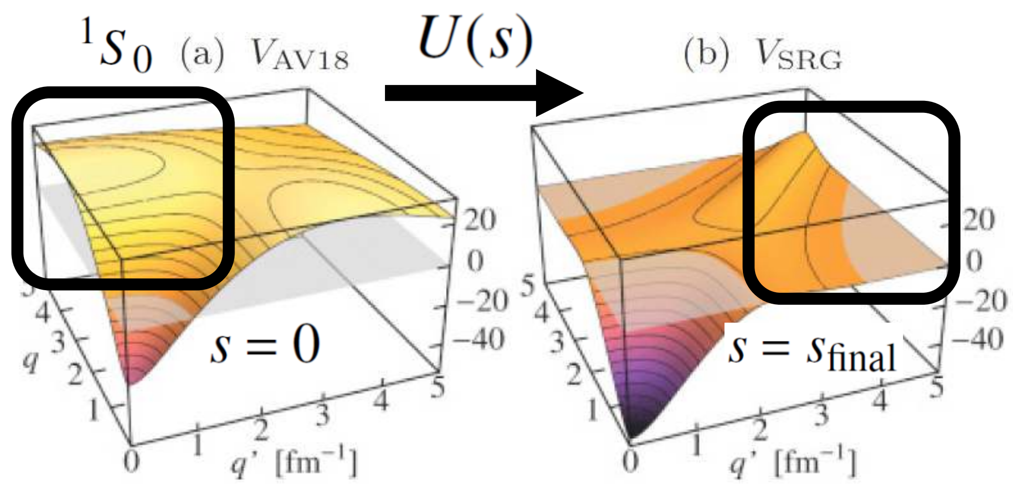
$$H(s) \equiv U(s) H U^\dagger(s)$$
$$= T + V^{2N}(s) + V^{3N}(s) + \dots$$

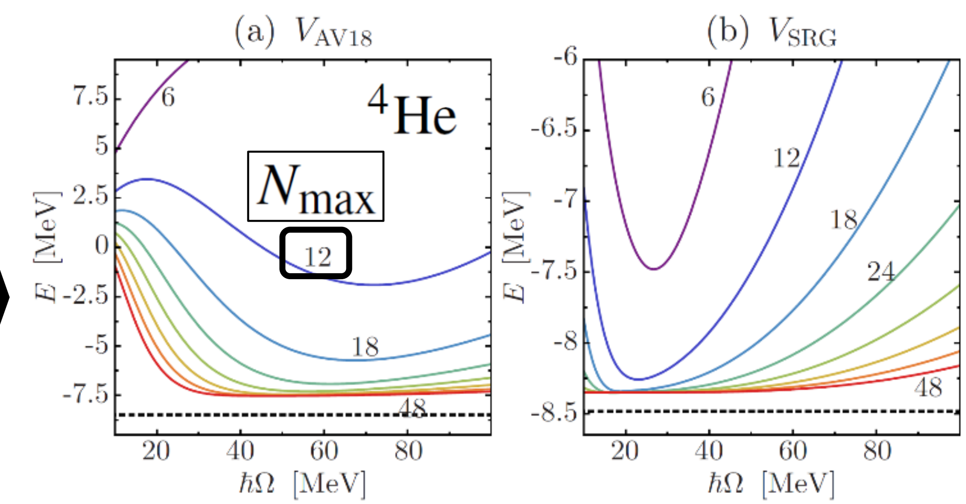
1) Unitary **Similarity Renormalization Group** (SRG) transformatior

$$\frac{dH(s)}{ds} = [\eta(s), H(s)]$$

with

$$\eta(s) = \frac{dU(s)}{ds} U^\dagger(s)$$
$$\equiv [T, H(s)]$$





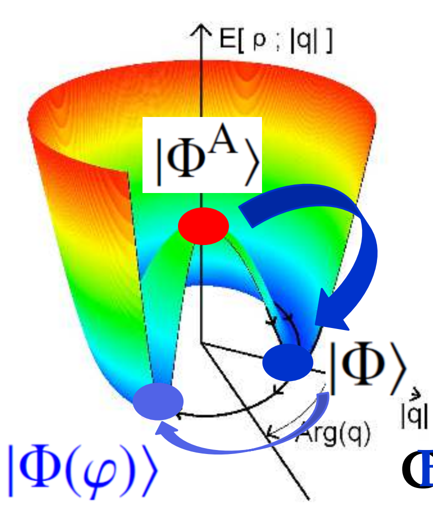
[Roth, Reinhardt, Hergert 2008]

$$V^{2N}(s)(q,q') \approx V^{2N}(0)(q,q') e^{-s(q^2-q'^2)^2}$$

Low-to-high off-diagonal matrix elements suppressed
But k-body operators induced…

Drastically accelerated convergence
Still ~2000 basis states needed in mid-mass
More perturbative behavior in the UV
Limit to SOS to utilize AMC → 200 states
Limit to « low » orders (CCSD(T), IMSRG(2), MBPT(3))
Limit to mid mass (A~8

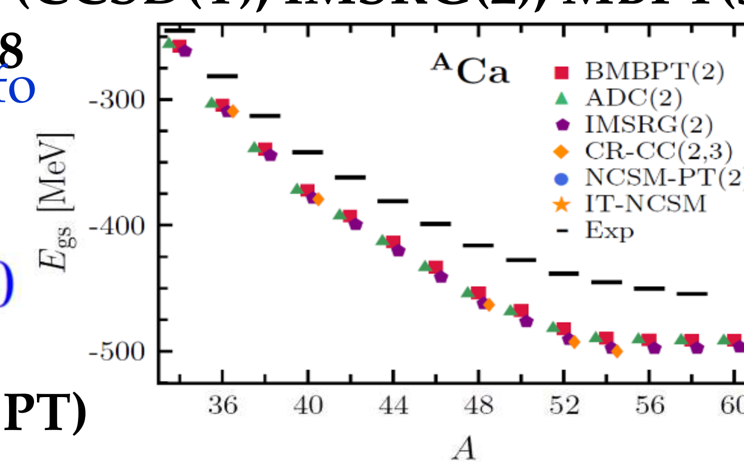
2) **Symmetry breaking** mean-field reference state
2a) U(1)-breaking Bogoliubov product state in SOS
2b) SU(2)-breaking Slater determinant in DOS



Slater determinant → ph degeneracy in OS
SB reference state commutes ph degeneracy into group transfo

Ex: MBPT
Ex: BMBPT

$$\Delta E^{(2)}_{MBPT} = -\frac{1}{4}\sum_{ijab} \frac{|H^{40}_{ijab}|^2}{e_a + e_b - e_i - e_j} \quad \frac{|{}_{k_3 k_4}|^2}{\dots = 0 + E_{k_4}} > 0$$



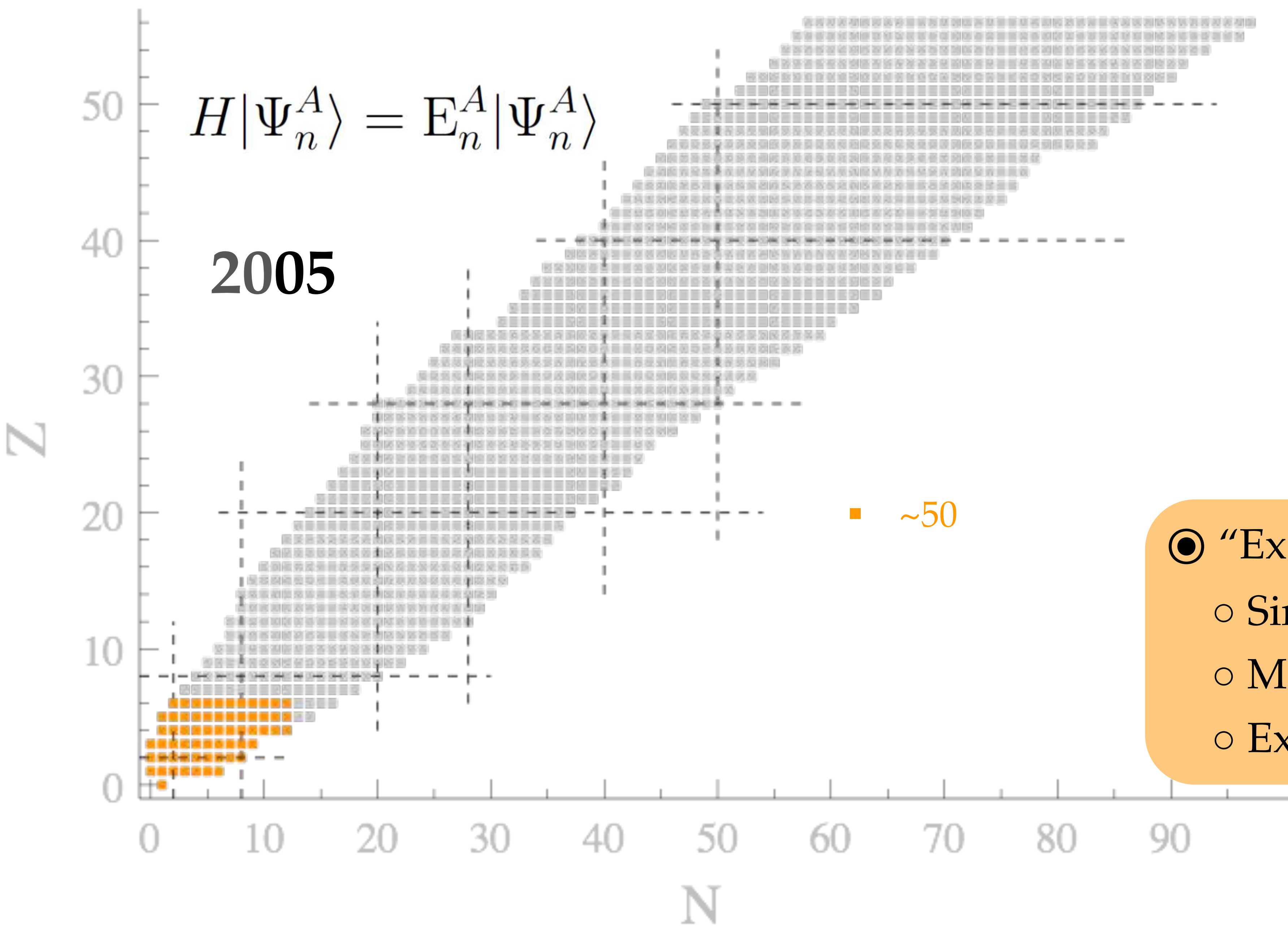
[Tichai et al. 2018]

Capture static correlations as MR methods (CPU/100 for BMBPT)
Broken symmetry must eventually be restored [Duguet 2015]
Singular expansion

Contents

- Introduction to low-energy nuclear physics
  - Phenomenology
  - Rationale from the theoretical viewpoint
- Strong inter-nucleon forces
  - Phenomenology and modern modelling
- The ab initio nuclear many-body problem
  - Specificities
  - Recent developments
  - Status of ab initio calculations of medium-mass atomic nuclei
- Conclusions and perspectives

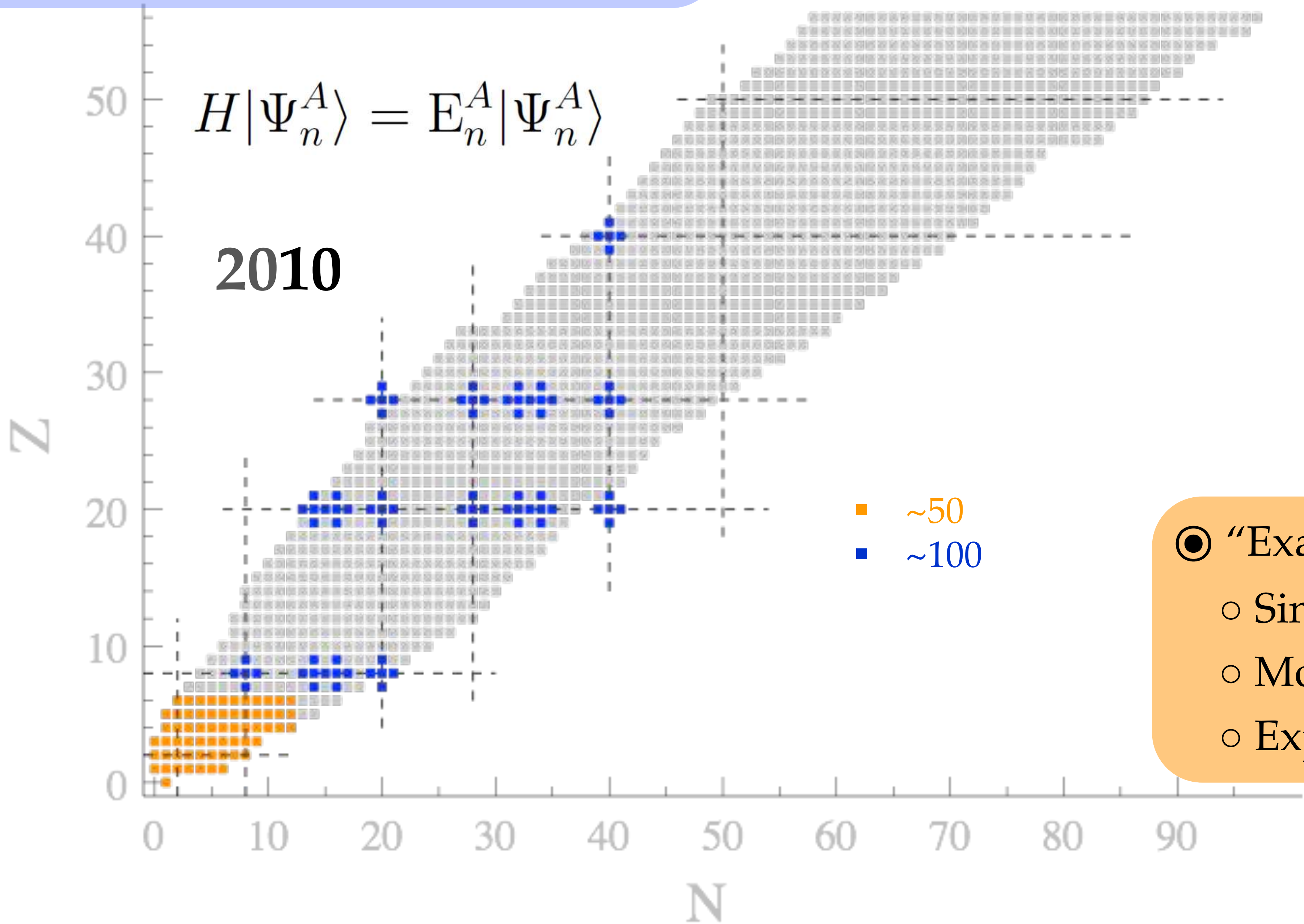
Evolution of ab initio nuclear chart



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

Evolution of ab initio nuclear chart

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

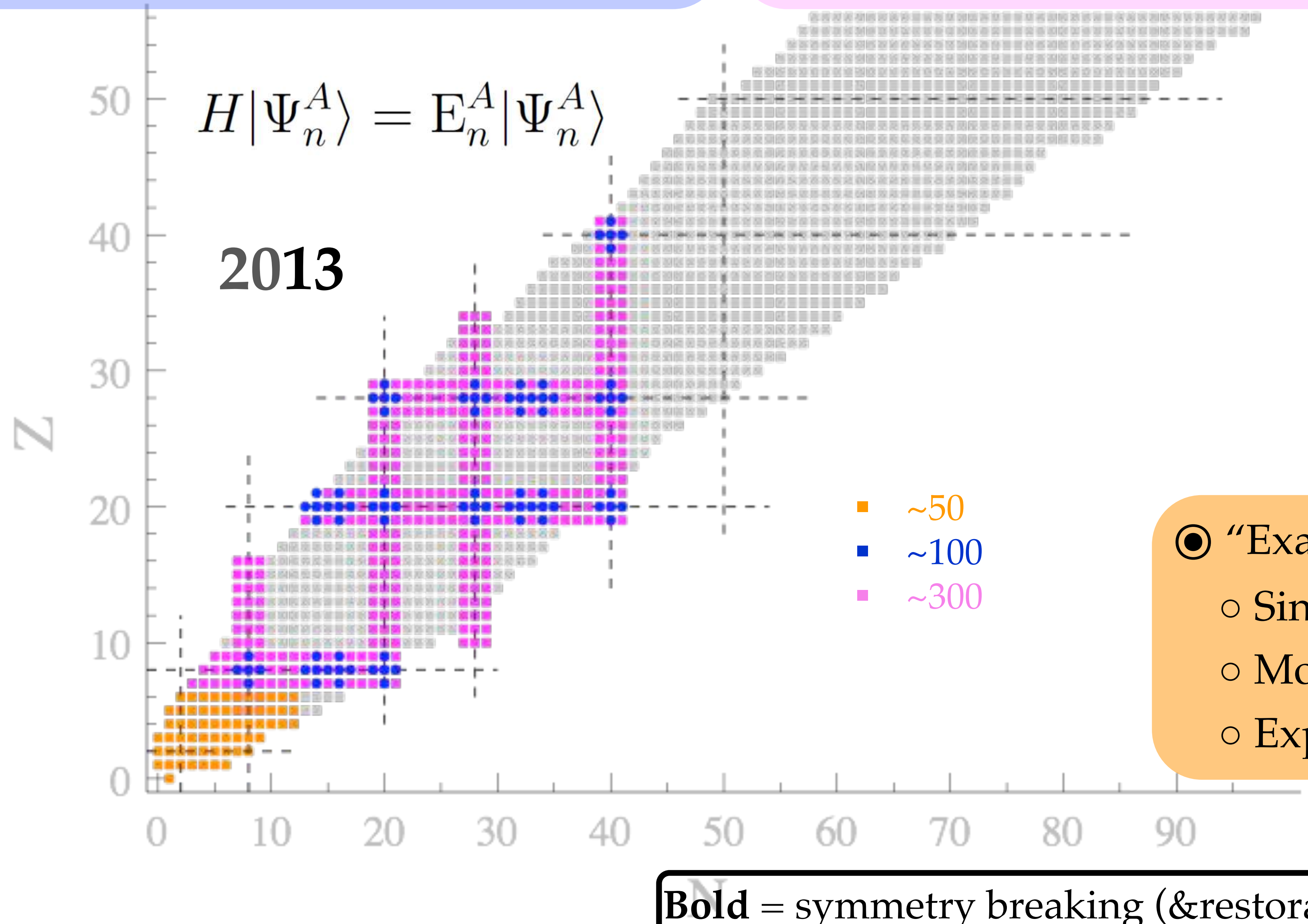


- ◉ "Exact" methods
  - ○ Since 1980's
  - ○ Monte Carlo, CI, …
  - ○ Exponential scaling

Evolution of ab initio nuclear chart

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

◉ Expansion methods for open-shells
- Since 2010's
- **(P)BMBPT**, **GSCGF**, **(P)BCC**, MR-IMSRG, MR-MBPT
- Polynomial scaling



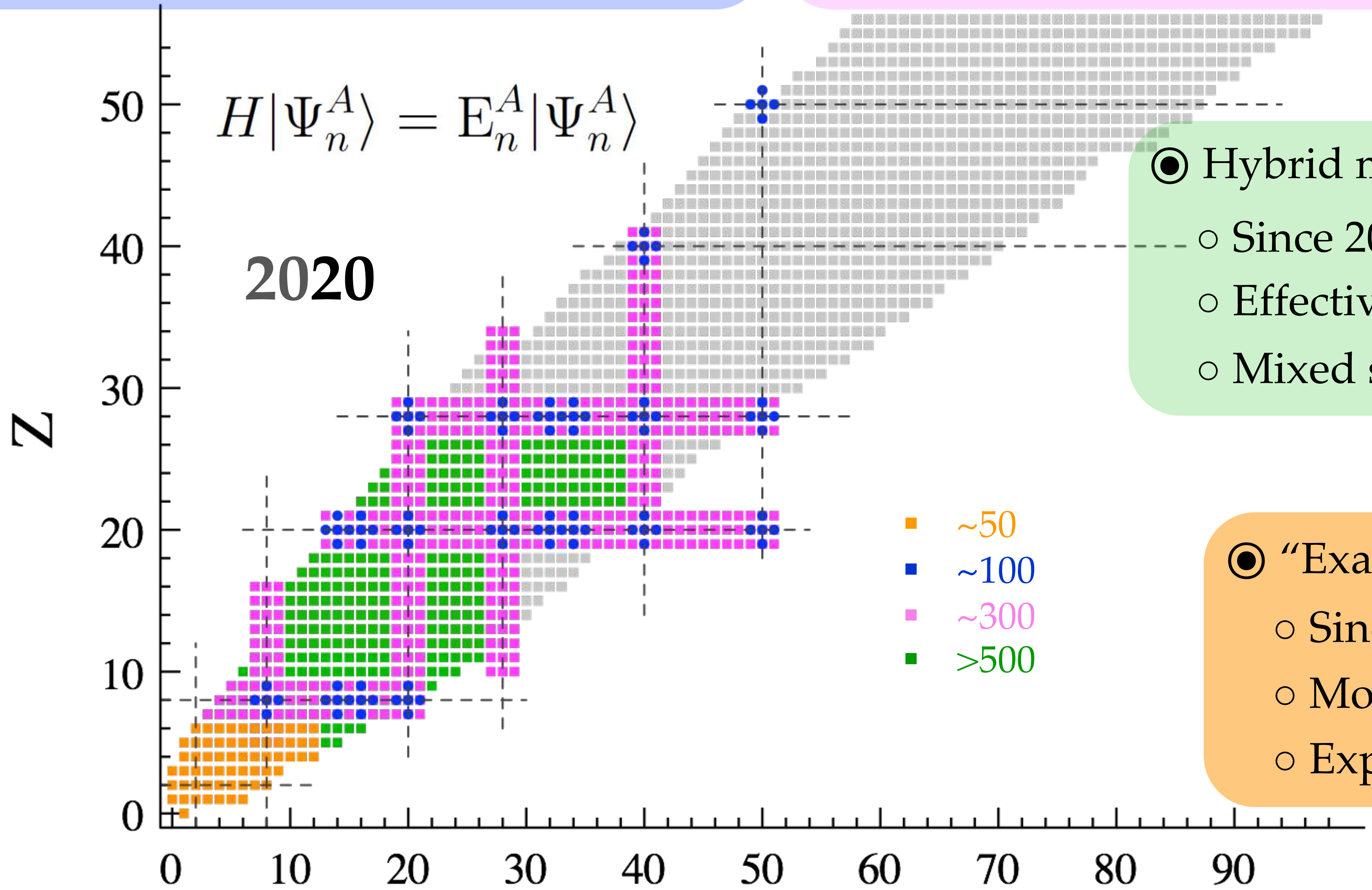
◉ "Exact" methods
- Since 1980's
- Monte Carlo, CI, …
- Exponential scaling

Bold = symmetry breaking (&restoration) single-reference methods

Evolution of ab initio nuclear chart

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

◉ Expansion methods for open-shells
- ○ Since 2010's
- ○ **(P)BMBPT**, **GSCGF**, **(P)BCC**, MR-IMSRG, MR-MBPT
- ○ Polynomial scaling



◉ 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

Bold = symmetry breaking (&restoration) single-reference methods

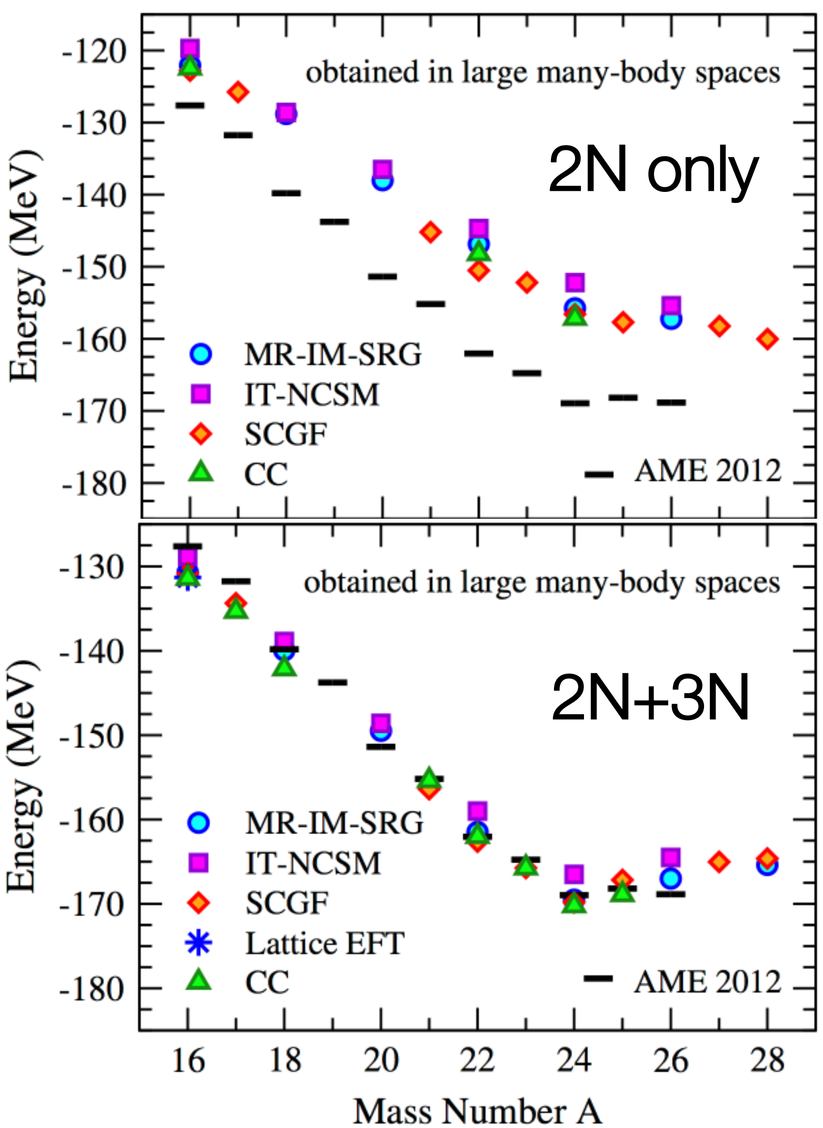
Contents

- ◉ Introduction to low-energy nuclear physics
  - ○ Phenomenology
  - ○ Rationale from the theoretical viewpoint
- ◉ Strong inter-nucleon forces
  - ○ Phenomenology and modern modelling
- ◉ The ab initio nuclear many-body problem
  - ○ Specificities
  - ○ Recent developments
  - ○ Status of ab initio calculations of medium-mass atomic nuclei
- ◉ Conclusions and perspectives

Oxygen binding energies

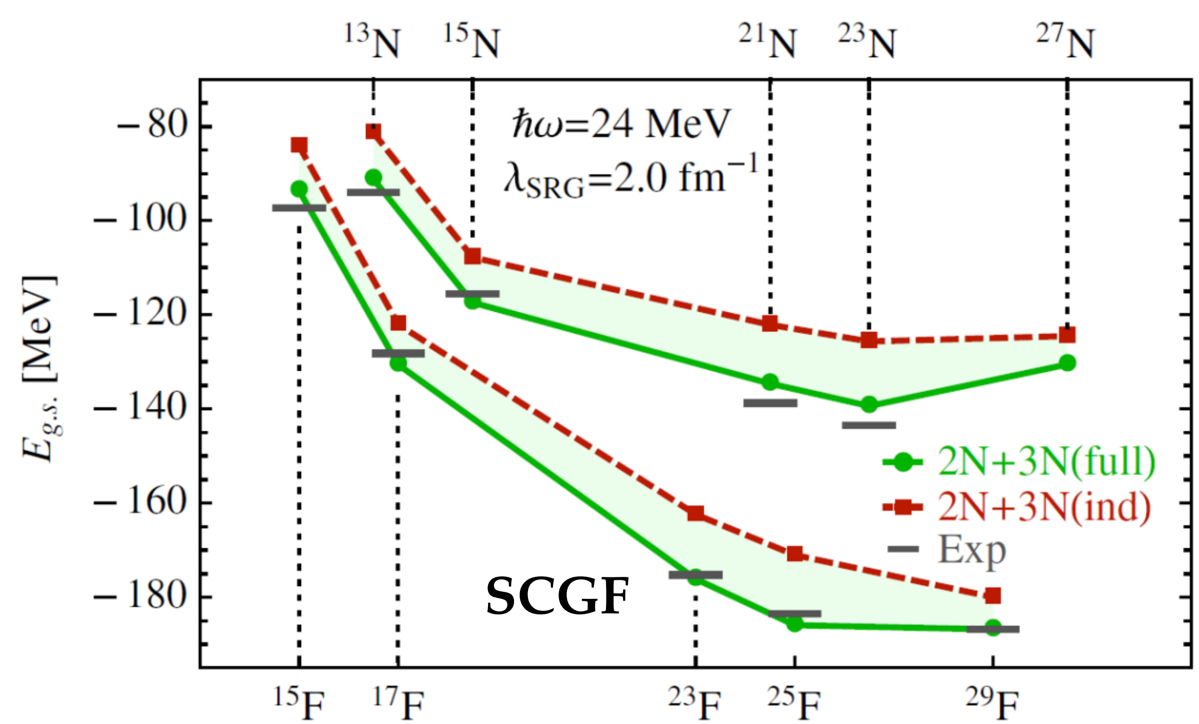
◉ Oxygen chain: importance of **three-body forces** and **benchmark** case for ab initio calculations

[Hebeler *et al.* 2015]



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

(Inconsistent) Chiral N^{3}LO 2N + N^{2}LO 3N interactions



[Cipollone, Barbieri, Navrátil 2013]

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

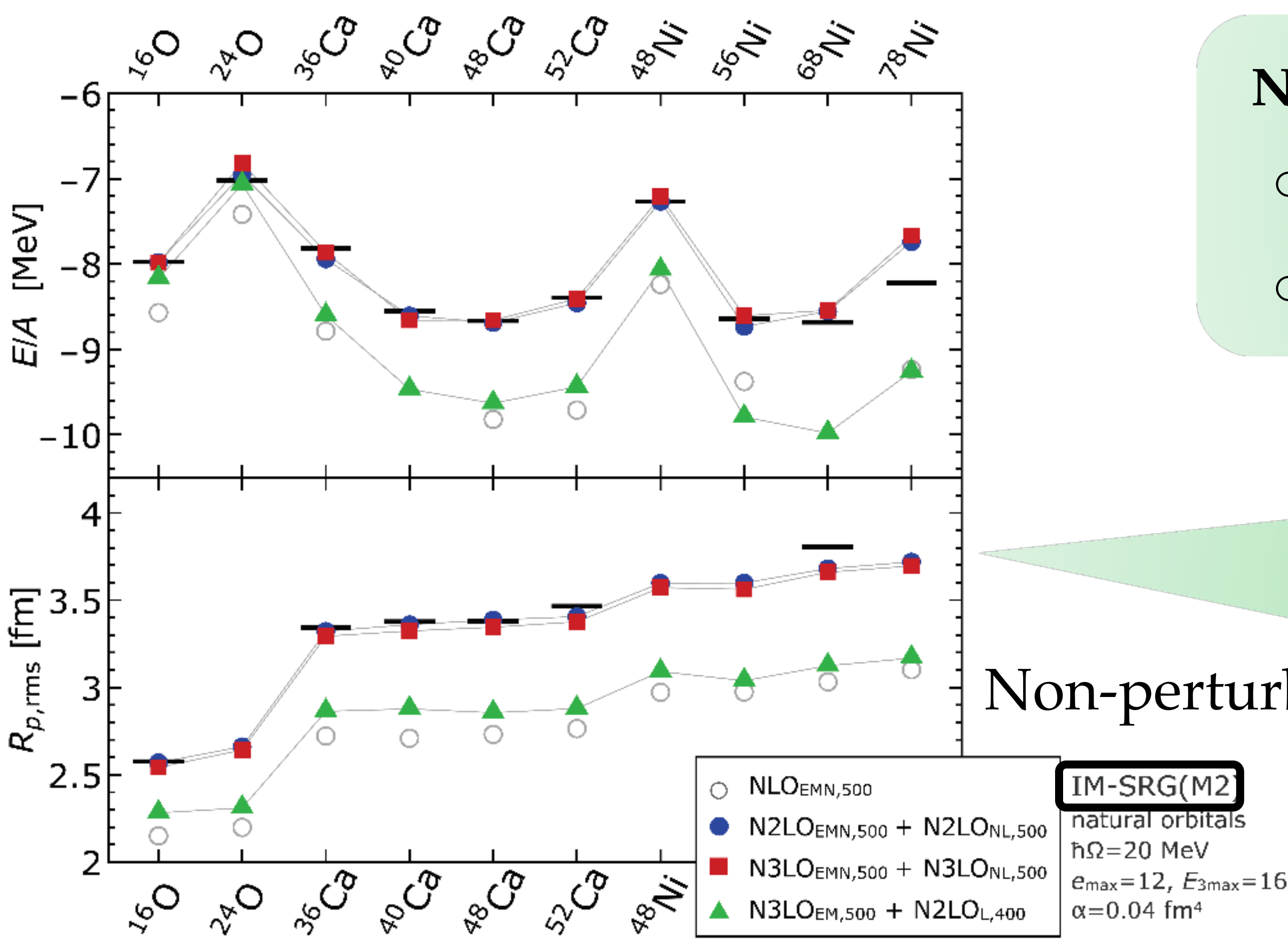
- ✓ All methods yield consistent results within 2-3%
- ✓ **3N interaction mandatory**
- ✓ Correct trend and drip-line location at N=16

Extension to radii and mid-mass doubly closed-shell nuclei

Situation pre-2019 **New situation**

[Huther *et al.* 2019]

[Huther *et al.* 2019]



New consistent chiral family at NLO, N²LO, N³LO

- ○ Non-local 3N regulator
- ○ C_D LEC tuned to BE(^{16}O) (^{4}He slightly relaxed)

- ○ **Excellent reproduction of binding energies**
- ○ **Excellent agreement for radii**
- ○ Net improvement from NLO to N²LO
- ○ Stable from N²LO to N³LO

Non-perturbative method

Successful **-ab initio description**
-of doubly closed-shell
-ground states
-up to A=78

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

Inconsistent Chiral N³LO 2N + N²LO 3N interactions

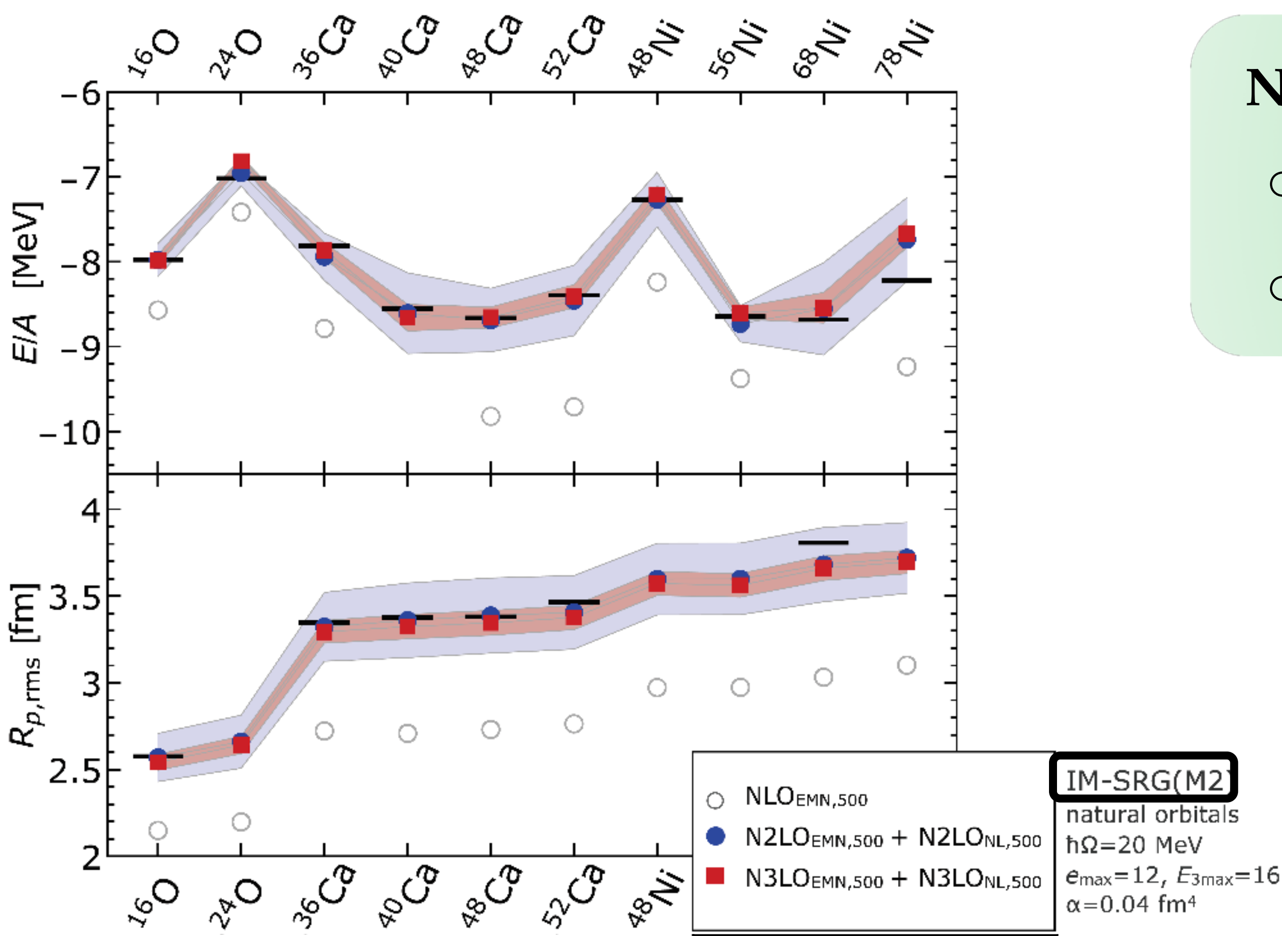
- ○ Overbinding beyond ^{A}O that increases with mass
- ○ Charge radii are consistently too small from ^{16}O till ^{78}Ni

Up to 20% error with data

Interaction uncertainties in doubly closed-shell nuclei

« Bare » results With uncertainties

[Huther *et al.* 2019]



[Huther *et al.* 2019]

New consistent chiral family at NLO, N²LO, N³LO

- Non-local 3N regulator
- C_D LEC tuned to BE(^{16}O) (^{4}He slightly relaxed)

Add interaction uncertainty

Order-by-order uncertainty from interaction

Simple protocol from expansion parameter Q/Λ_χ

Ex:

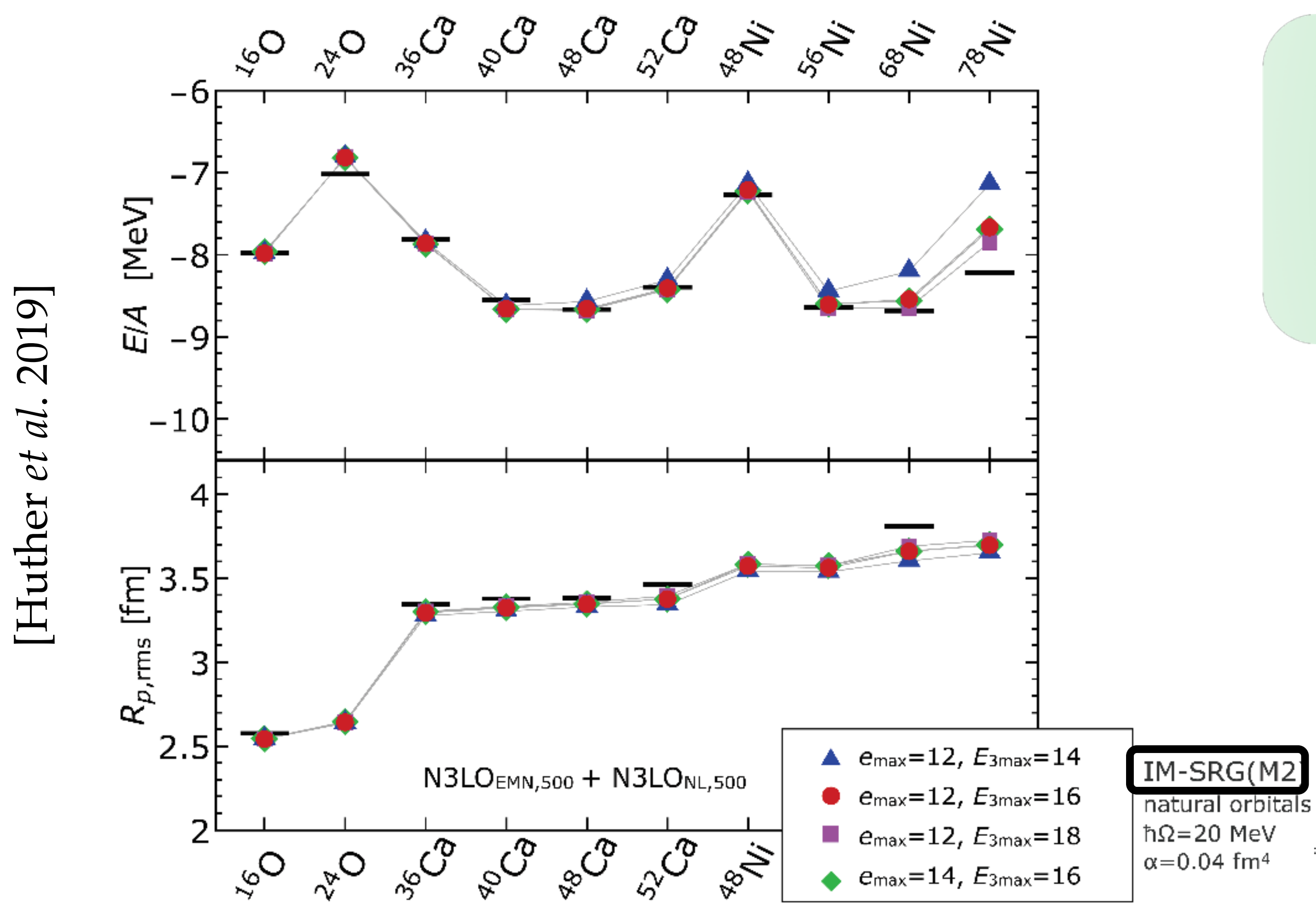
$$\delta O_{N^3LO} = \text{Max}\left\{ \left(\frac{Q}{\Lambda_\chi}\right)|O_{N^3LO} - O_{N^2LO}| \quad \left(\frac{Q}{\Lambda_\chi}\right)^2 |O_{N^2LO} - O_{NLO}| \quad \left(\frac{Q}{\Lambda_\chi}\right)^4 |O_{NLO} - O_{LO}| \quad \left(\frac{Q}{\Lambda_\chi}\right)^5 |O_{LO}| \right\}$$

- Consistent results from N²LO to N³LO
- **BE and radii uncertainty at N³LO: ~5-6%**
- More refine estimate possible and envisioned

Many-body uncertainties in doubly closed-shell nuclei

« Bare » results   With uncertainties

[Huther *et al*. 2019]



New consistent chiral family at NLO, N^2LO, N^3LO

- ○ Non-local 3N regulator
- ○ C_D LEC tuned to BE(^{16}O) (^{4}He slightly relaxed)

Add basis uncertainty

Harmonic Oscillator basis uncertainty

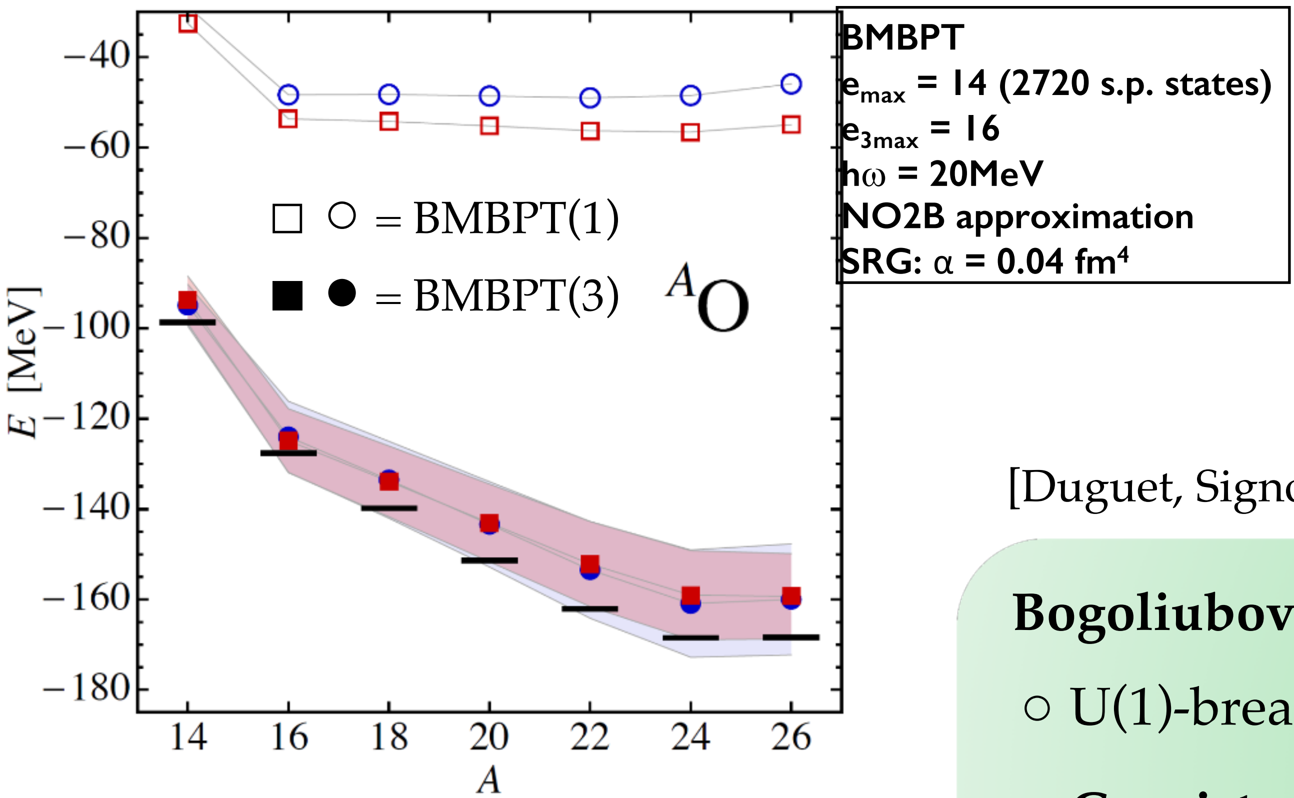
Increase bases to represent 2N and 3N tensors

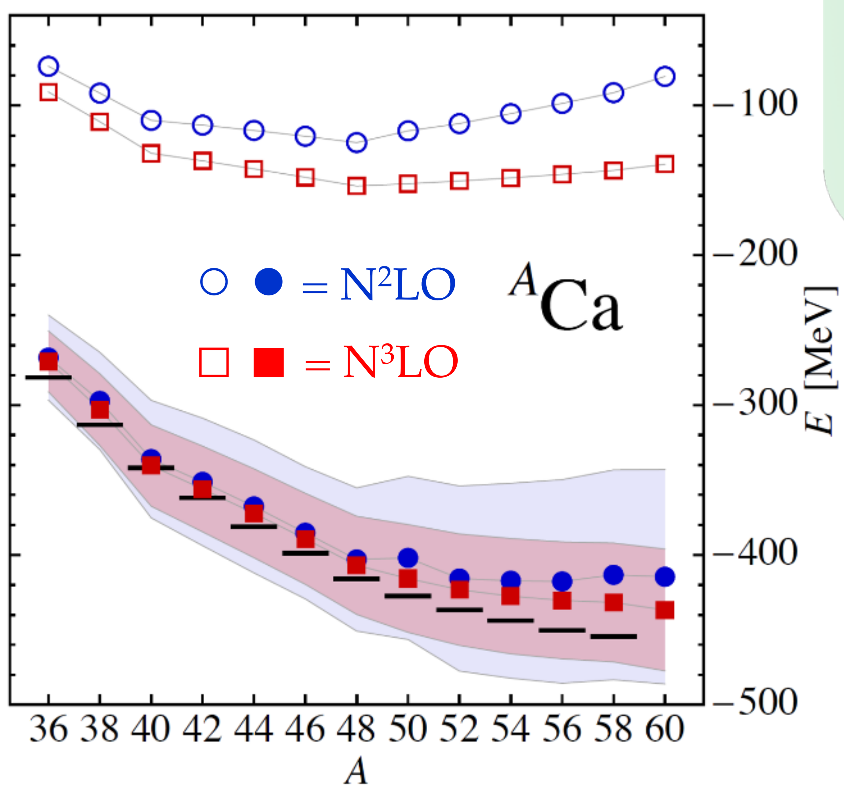
+ omitted SRG-induced k-body forces beyond k=3
+ NO2B approximation to the 3N operator
+ truncation of many-body expansion

- ○ **Fully converged calculations with respect basis size in mid mass nuclei**
  - ○ Challenge however to go to heavier systems and refined many-body truncations
- ○ **Total many-body uncertainty in mid-mass nuclei ~2-3%** dominated by NO2B approximation
- ○ **Uncertainty in mid-mass systems dominated by truncation in chiral EFT expansion**

Binding energy in singly open-shell nuclei

[Tichai, Roth, Duguet 2020]





[Huther *et al*. 2019]

New consistent chiral family at NLO, N²LO, N³LO

- ○ Non-local 3N regulator
- ○ C_D LEC tuned to BE(^{16}O) (^{4}He slightly relaxed)

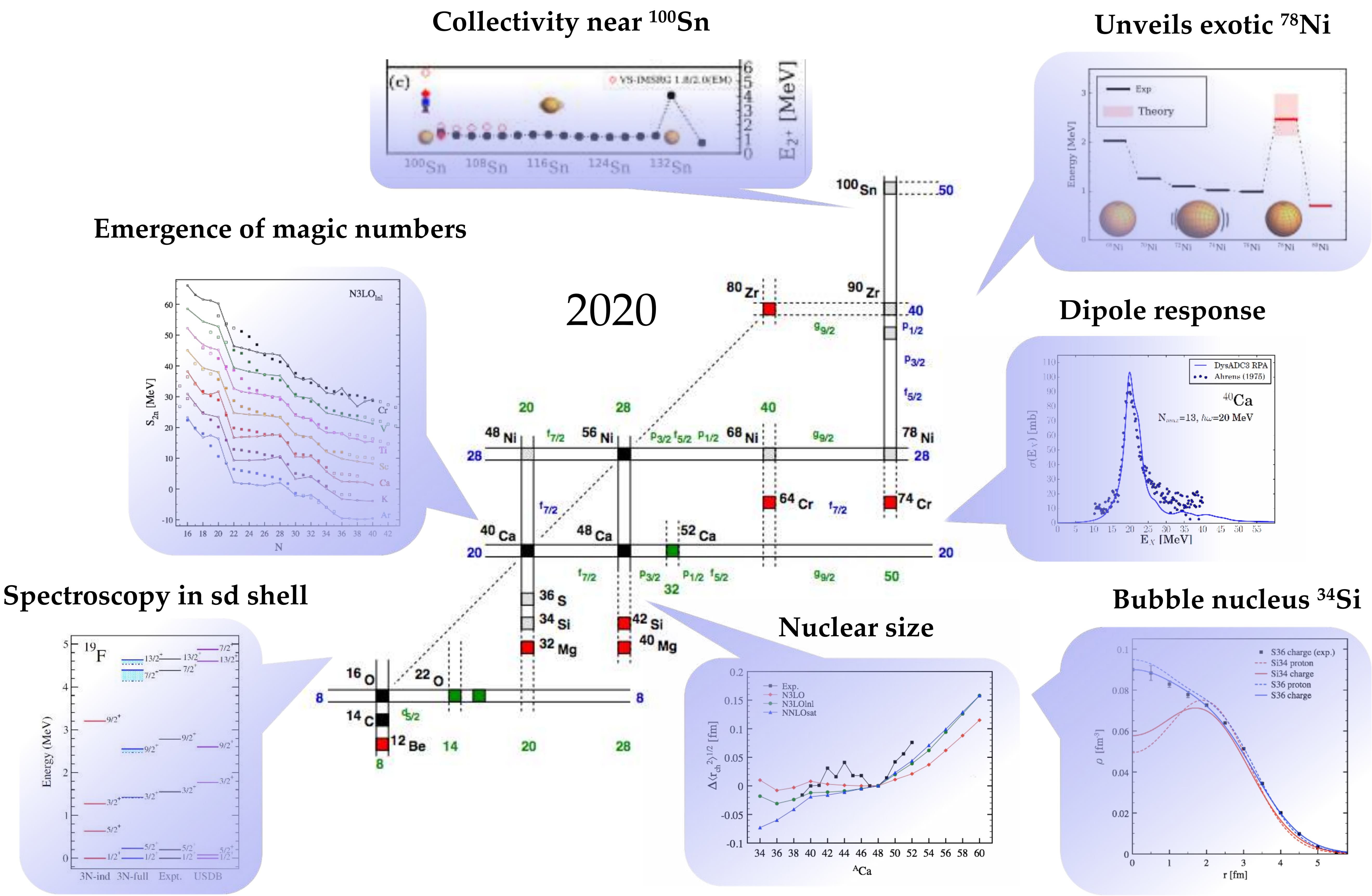
[Duguet, Signoracci 2016; Tichai *et al* 2018]

Bogoliubov many-body perturbation theory

- ○ U(1)-breaking Bogoliubov (HFB) reference state
- ○ **Consistent with non-perturbative methods to 2-3%**
- ○ CPU/100 = ideal for large-scale studies
- ○ **Symmetry to be restored = PBMBPT (PCC)** [Duguet, Signoracci 2016]

- ○ **Estimated error from BMBPT(>3) below 2%** (not correct on the Fig.)
- ○ **Consistent results with closed-shell results**
  - ○ Agreement with data much improved compared to pre-2019
  - ○ Uncertainty dominated by interaction (less true in neutron rich Ca)

Nuclear structure features addressed ab initio



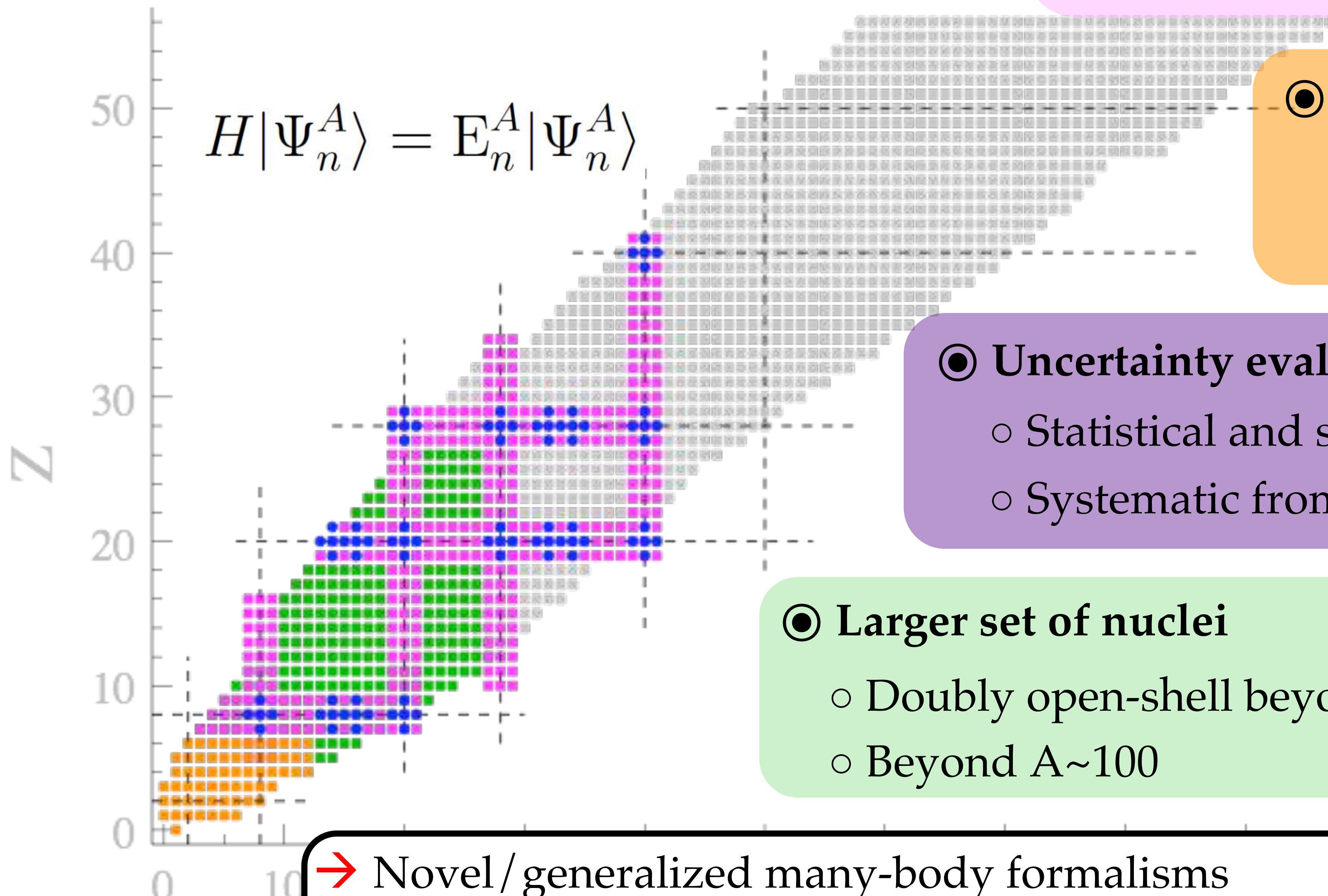
Some challenges for ab initio theory

◉ 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

- Introduction to low-energy nuclear physics
  - Phenomenology
  - Rationale from the theoretical viewpoint
- Strong inter-nucleon forces
  - Phenomenology and modern modelling
- The ab initio nuclear many-body problem
  - Specificities
  - Recent developments
  - Status of ab initio calculations of medium-mass atomic nuclei
- Conclusions and perspectives

General conclusions

◉ Enormous progress of nuclear 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

Recent/on-going cross-fertilization between nuclear physics and quantum chemistry

1) Symmetry breaking and restored methods: NP → QC

BMBPT/BCC

[A. Signoracci, T. Duguet, G. Hagen, G. R. Jansen, Phys. Rev. C91 (2015) 064320]

[**T. M. Henderson, G. E. Scuseria**, J. Dukelsky, A. Signoracci, T. Duguet, Phys. Rev. C89 (2014) 054305]

PBMBPT/PBCC

[T. Duguet, J. Phys. G: Nucl. Part. Phys. 42 (2015) 025107]

[**Y. Qiu, T. M. Henderson,** T. Duguet, **G. E. Scuseria**, Phys. Rev. C99 (2019) 044301]

2) Multi-reference methods: QC → NP

MRMBPT

[**Z. Rolik, A. Szabados, P. R. Surján**, J. Chem. Phys. 119 (2003) 1922]

[A. Tichai, E. Gebrerufael, K. Vobig, R. Roth, Phys. Lett. B786 (2018) 448]

3) In-medium similarity renormalization group method: NP → QC

[K. Tsukiyama, S. K. Bogner, A. Schwenk, Phys. Rev. Lett. 106 (2011) 222502]

[A. Tichai, **J. Toulouse, E. Giner** , T. Duguet, work in progress]

4) Tensor-factorization techniques: QC → NP

[**R. Schutski, J. Zhao, T. M. Henderson, G. E. Scuseria**, J. Chem. Phys. 147 (2017) 184113]

[A. Tichai, **R. Schutski, G. E. Scuseria**, T. Duguet, Phys. Rev. C99 (2019) 034320]

5) Importance truncation techniques for, e.g., (P)(B)CC: QC → NP

[**J. E. Deustua, J. Shen, P. Piecuch,** PRL 119 (2017) 223003]

[A. Tichai, J. Ripoche, T. Duguet, Eur. Phys. J. A55 (2019) 90]

Collaborators on ab initio many-body calculations

CEA
L. Contessi
J.-P. Ebran
M. Frosini
A. Porro
F. Raimondi
J. Ripoche
V. Somà

University of Surrey
P. Arthuis
C. Barbieri
M. Drissi

The University of Tennessee / Oak Ridge National Laboratory
G. Hagen
T. Papenbrock

NSCL
H. Hergert
R. Wirth

Rice
T. M. Henderson
Y. Qiu
G. E. Scuseria

TRIUMF
P. Navratil

Technische Universität Darmstadt
R. Roth
A. Tichai

KU Leuven
P. Demol

Back up slides

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

Elementary facts and « big » questions about nuclei

○ 252 **stable** isotopes, ~3100 synthesized in the lab

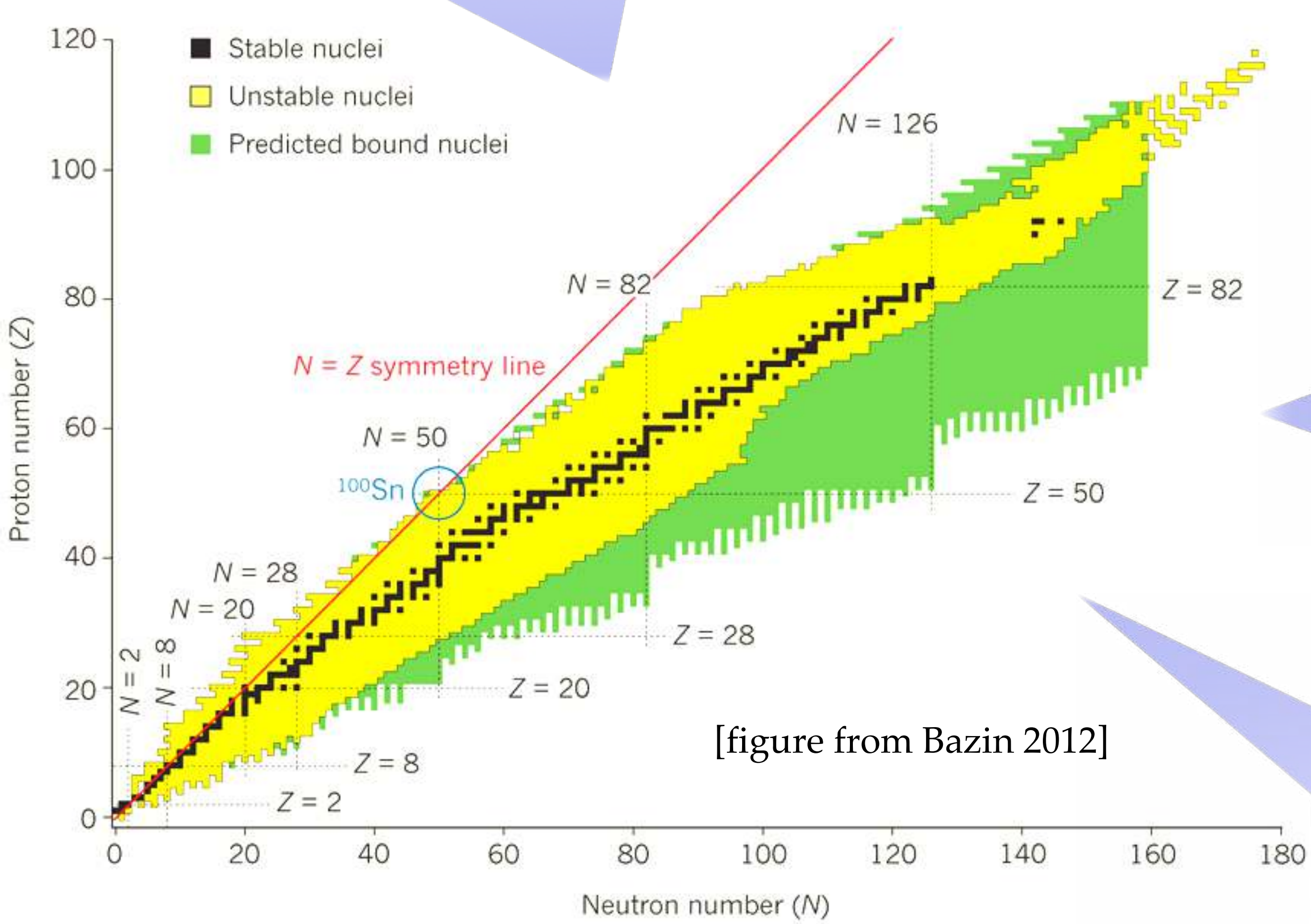
○ **How many** bound (w.r.t strong force) nuclei exist; 9000?

Oganesson ($_{118}$Og) added to Mendeleïev table in 2016

○ **Heaviest** synthesized element Z=118

○ **Heaviest possible** element?

○ Enhanced stability near Z=120?126?



[figure from Bazin 2012]

○ Modes of **instability** (α, β, γ decays, fission)

○ Are there more exotic decay modes?

○ Ex: ν-less 2β decay = test of standard model

○ Ex: 2p decay beyond the proton drip line

○ Elements **up to Fe** produced in stellar fusion

○ How have heavier elements been produced?

○ r-process nucleosynthesis in neutron star mergers

Updated in 2019 to Z=9 (22 neutrons) and Z=10 (24 neutrons)

○ Neutron **drip-line** known up to ~~Z=8 (16 neutrons~~)

○ Where is the neutron drip-line beyond Z=10?

○ Over-stable "magic" nuclei (2, 8, 20, 28, 50, 82, …)

○ Are **magic numbers** the same for unstable nuclei?

Single-reference expansion many-body methods

Nuclear Hamiltonian

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

Symmetry group

U(1) dealt with today

$$[H,S] = 0 \quad \text{where} \quad S \equiv \boxed{A}, J^2, J_z \ldots$$

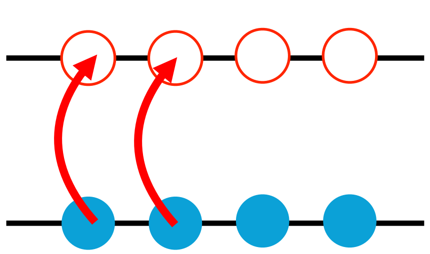
Mean-field reference state

$$H = H_0 + H_1 \quad \text{such that} \quad [H_0,S] = 0, \quad [H_1,S] = 0$$

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

Exactly solvable

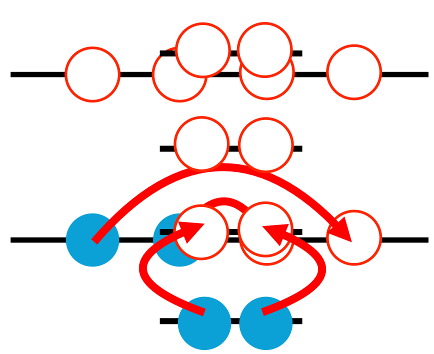
Closed-shell



Non-degenerate

Good starting point

Open-shell



Non-degenerate

Degenerate

Improper starting point

Proper starting point

A-body eigenvalue problem

$$H|\Psi_0^S\rangle = E_0^S|\Psi_0^S\rangle$$

N^A cost where N = dim H_1

Many-body expansion

$$H = H_0 + H_1$$

$$|\Psi_0^S\rangle = \underline{U^S(\infty)}\,\underline{|\Phi_0^S\rangle}$$

Wave operator — Reference state

- ▶ Accounts for « weak / dynamical » correlations
- ▶ Expand as a series (MBPT, CC…) + truncate = N^p cost

Symmetry breaking

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

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

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

$$|\Psi_0^S\rangle = \underline{U(\infty)}\,\underline{|\Phi_0\rangle}$$

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**

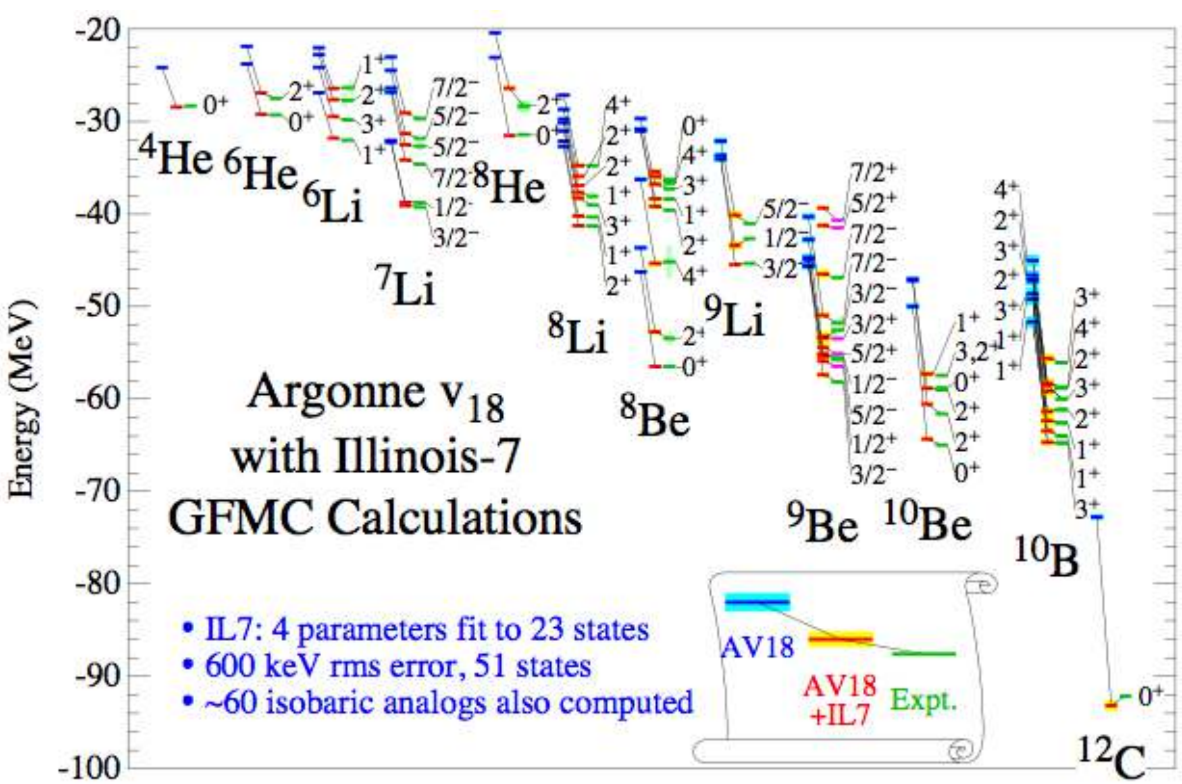
First ab initio calculations

➪ **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 (i.e. full CI)** [Vary, Barrett, Navratil, Ormand…]

- Diagonalisation of the Hamiltonian in a finite-dimensional space



Nuclei simulated from "scratch"!

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

[Pieper & Wiringa 2001]

✗ 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)**

Chiral EFT hamiltonians

◉ **N3LO (~2010)** [Entem & Machleidt 2003, Navrátil 2007, Roth et al. 2012]

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

SRG λ=2.0 fm^{-1}

◉ **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**

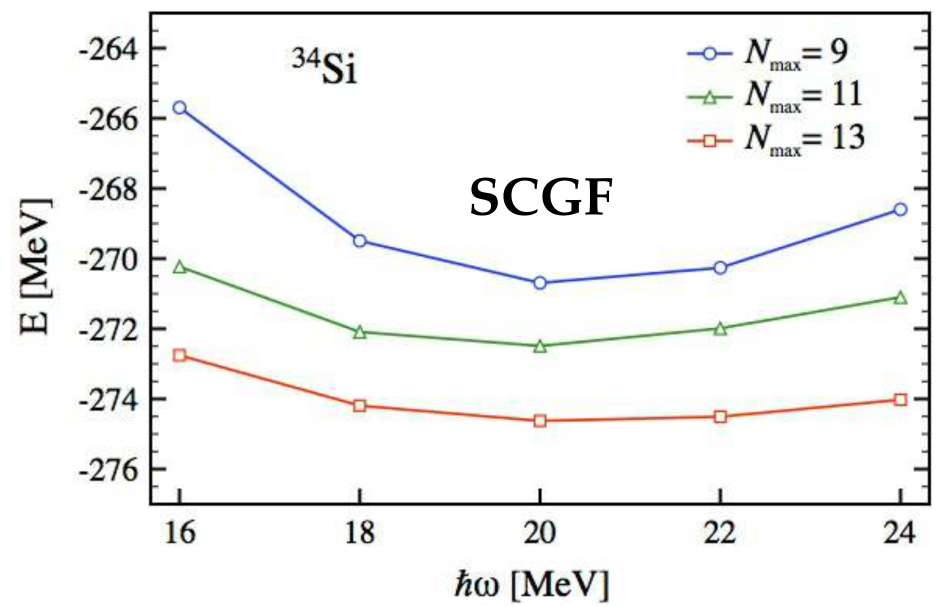
◉ **N3LO$_{lnl}$ (2018)** [Entem & Machleidt 2003, Navrátil 2018]

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

SRG λ=2.0 fm^{-1}

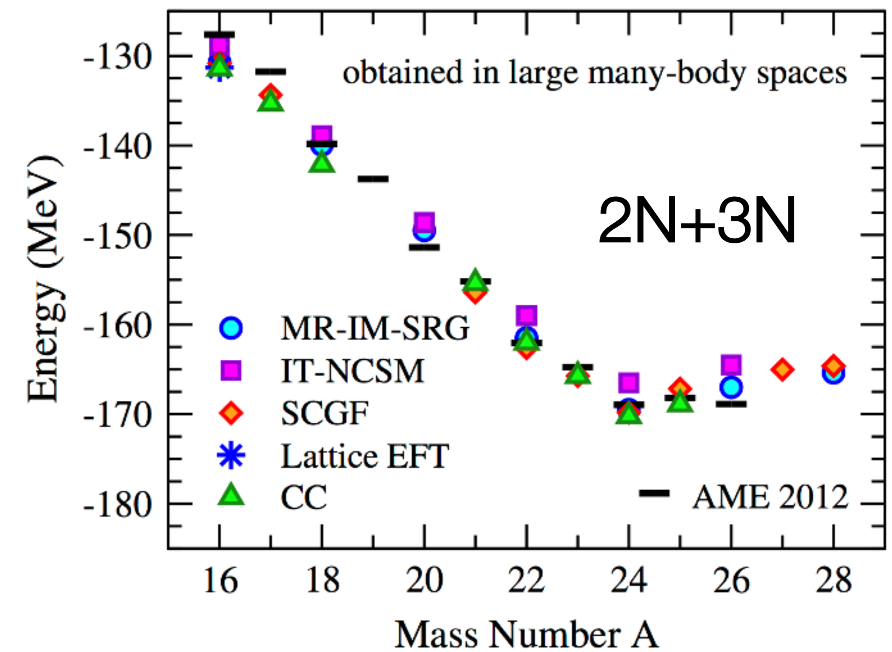
Sources of uncertainty

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



[Duguet et al. 2016]

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

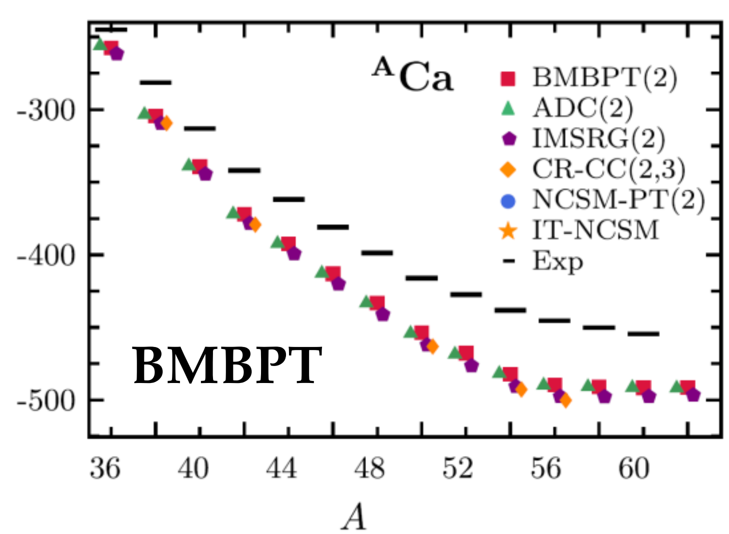


[Hebeler et al. 2015]

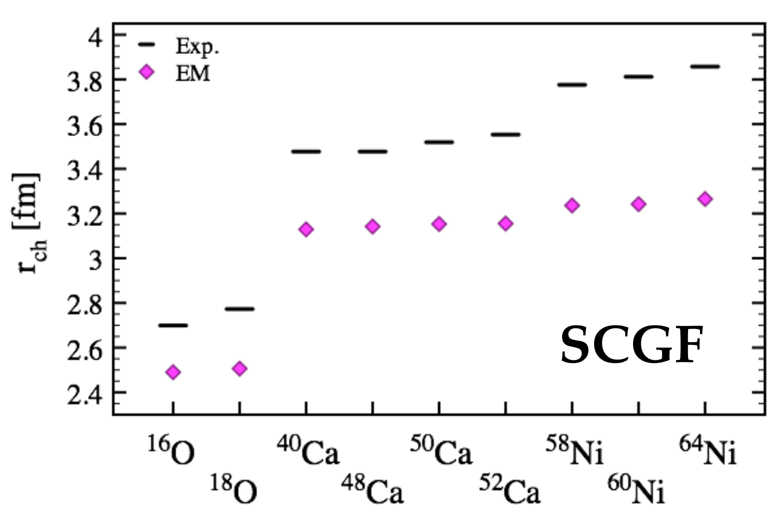
◉ **Difference with data up to 10-15% in Ca-Ni region with N3LO**

Energy

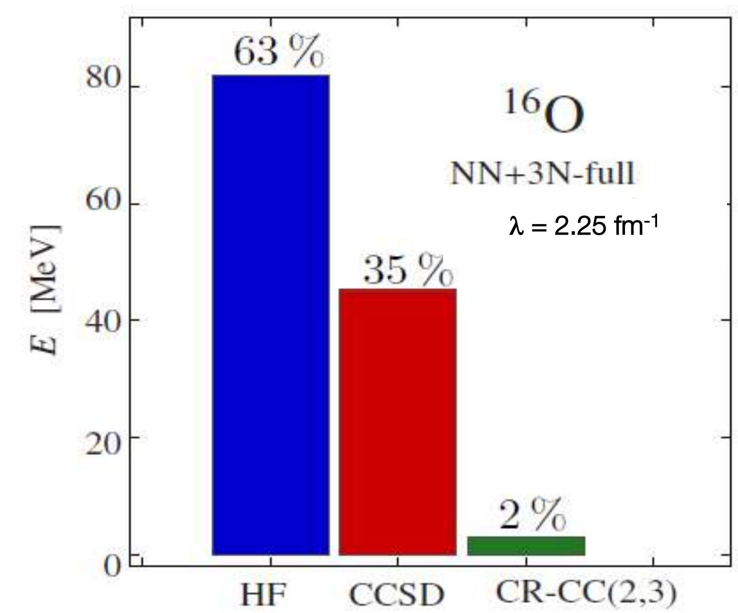
[Tichai et al. 2018]



Charge radius



[Somà, *et al.* 2019]



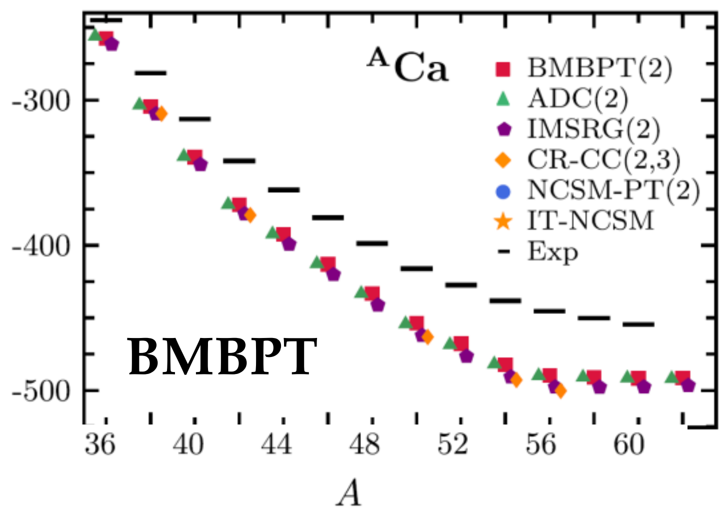
[Binder et al. 2015]

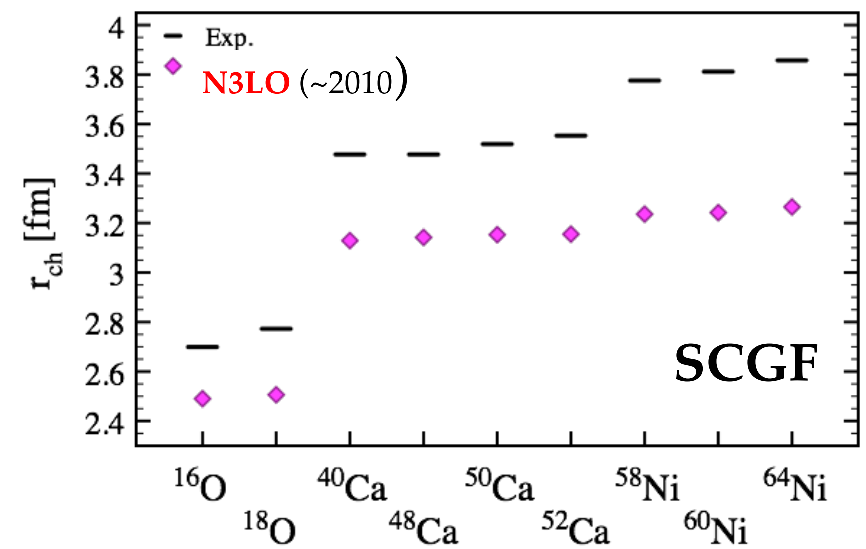
Largest uncertainty from input Hamiltonian

→ **Improved Hamiltonians needed**

Charge radii in medium-mass nuclei

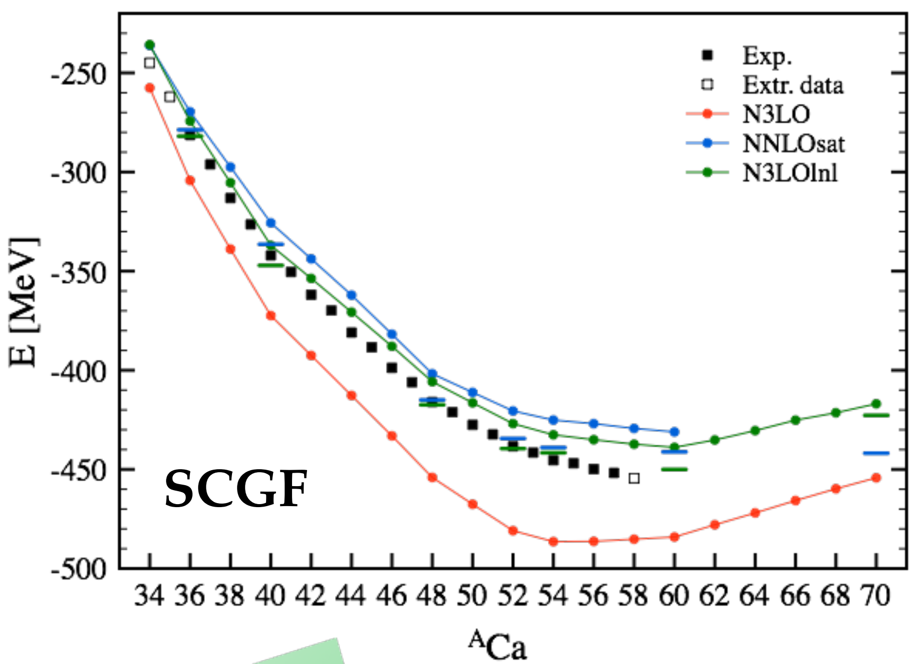
◉ **N3LO** (~2010)

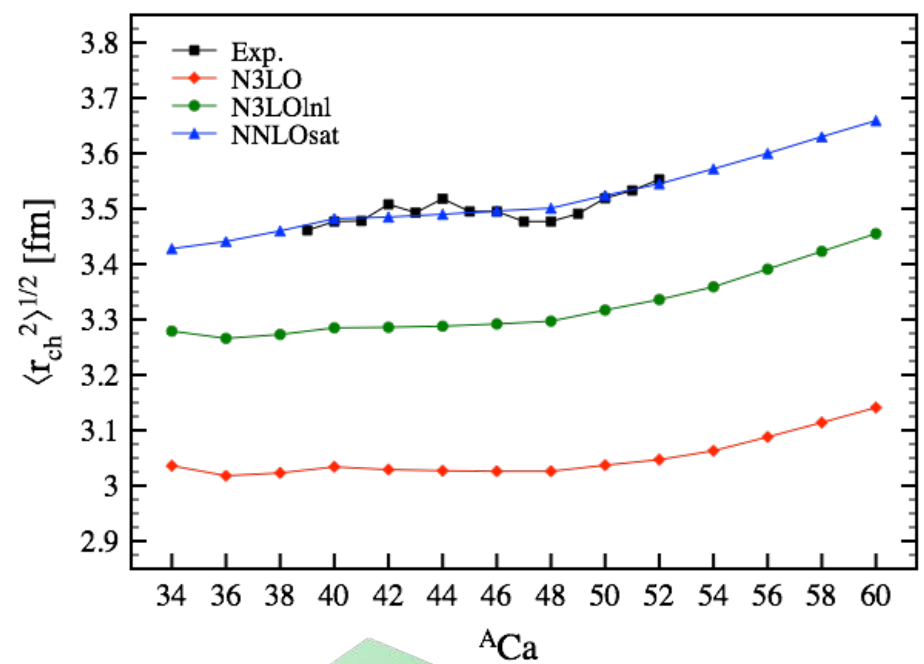




[Somà *et al.* 2019]

◉ Newly developed Hamiltonians improves the situation





[Somà *et al.* 2019]

○ New interactions correct for overbinding

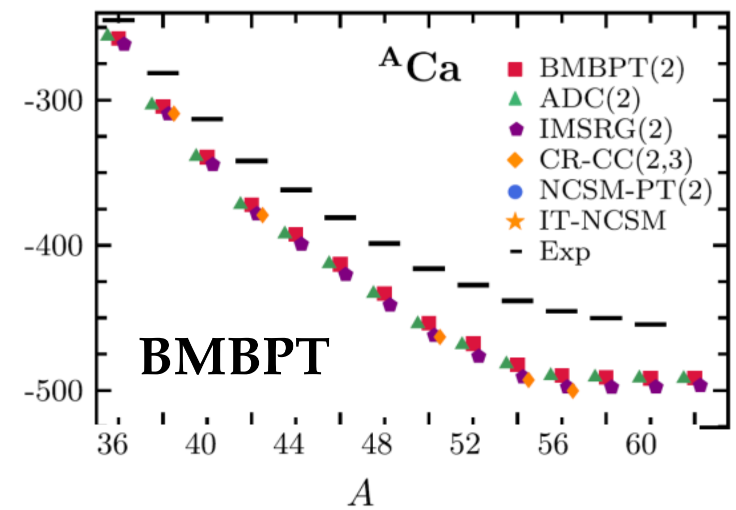
○ Full correlations needed

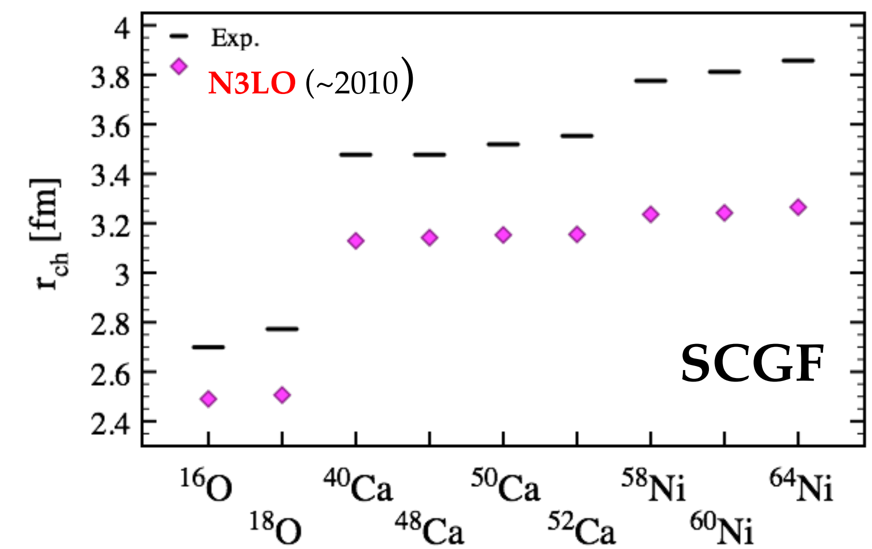
○ Radii OK when fitted!

○ Considerable improvement N3LO → N3LOlnl

Charge radii in medium-mass nuclei

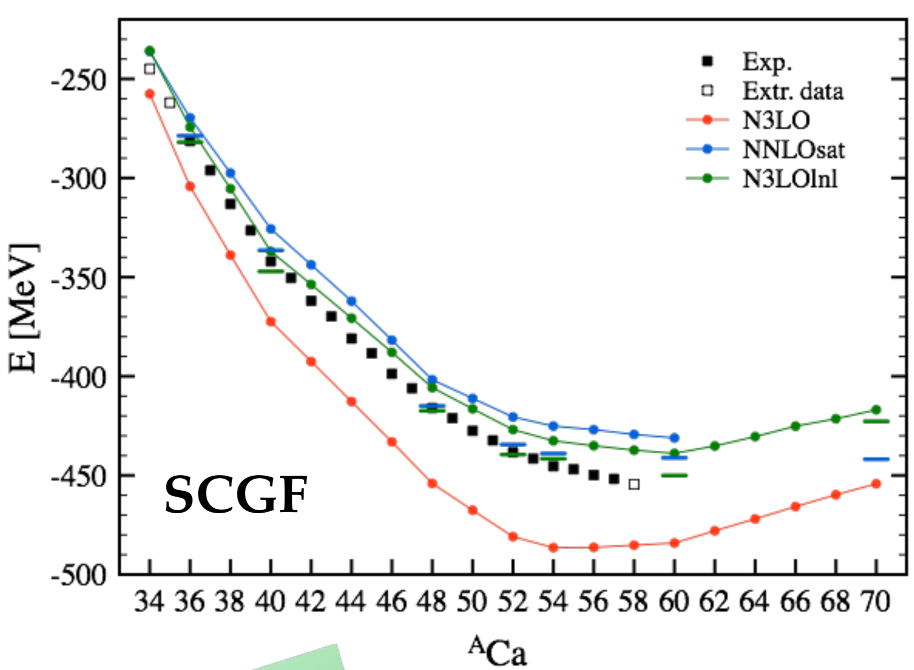
◉ **N3LO** (~2010)



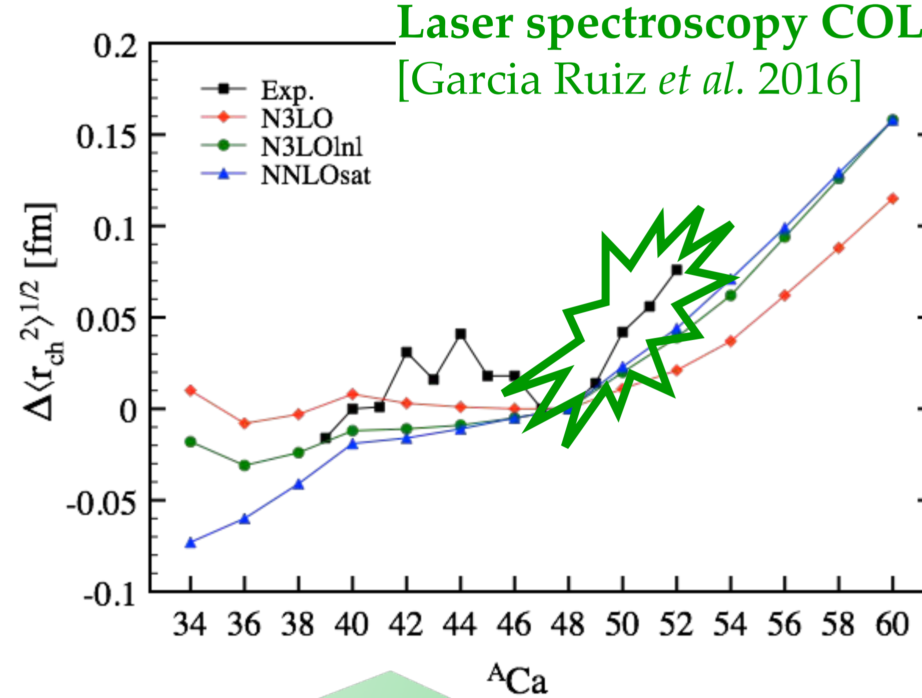


[Somà *et al.* 2019]

◉ Newly developed Hamiltonians improves the situation



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



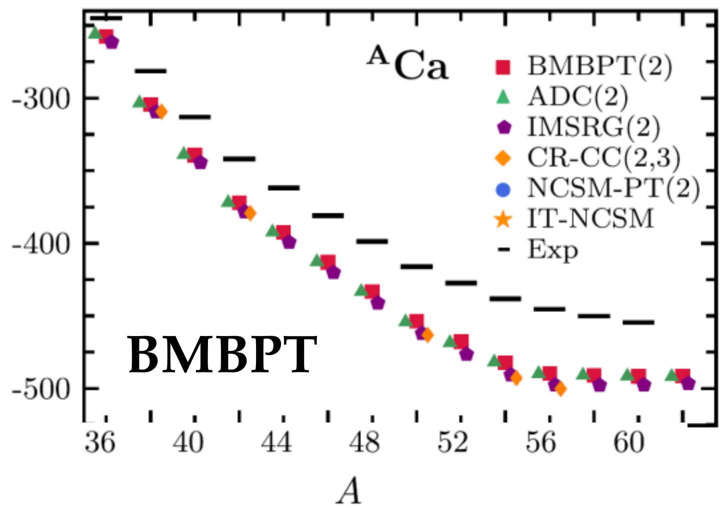
[Somà *et al.* 2019]

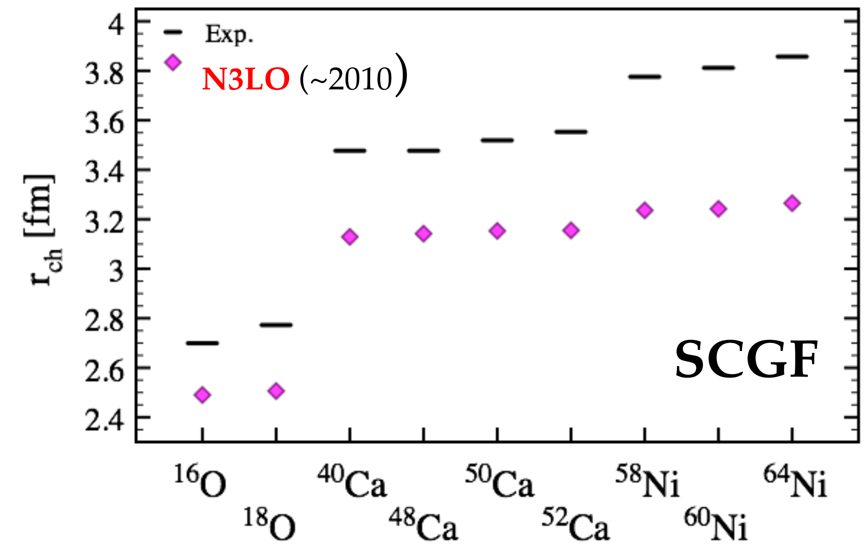
- ○ New interactions correct for overbinding
- ○ Full correlations needed

- ○ 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)

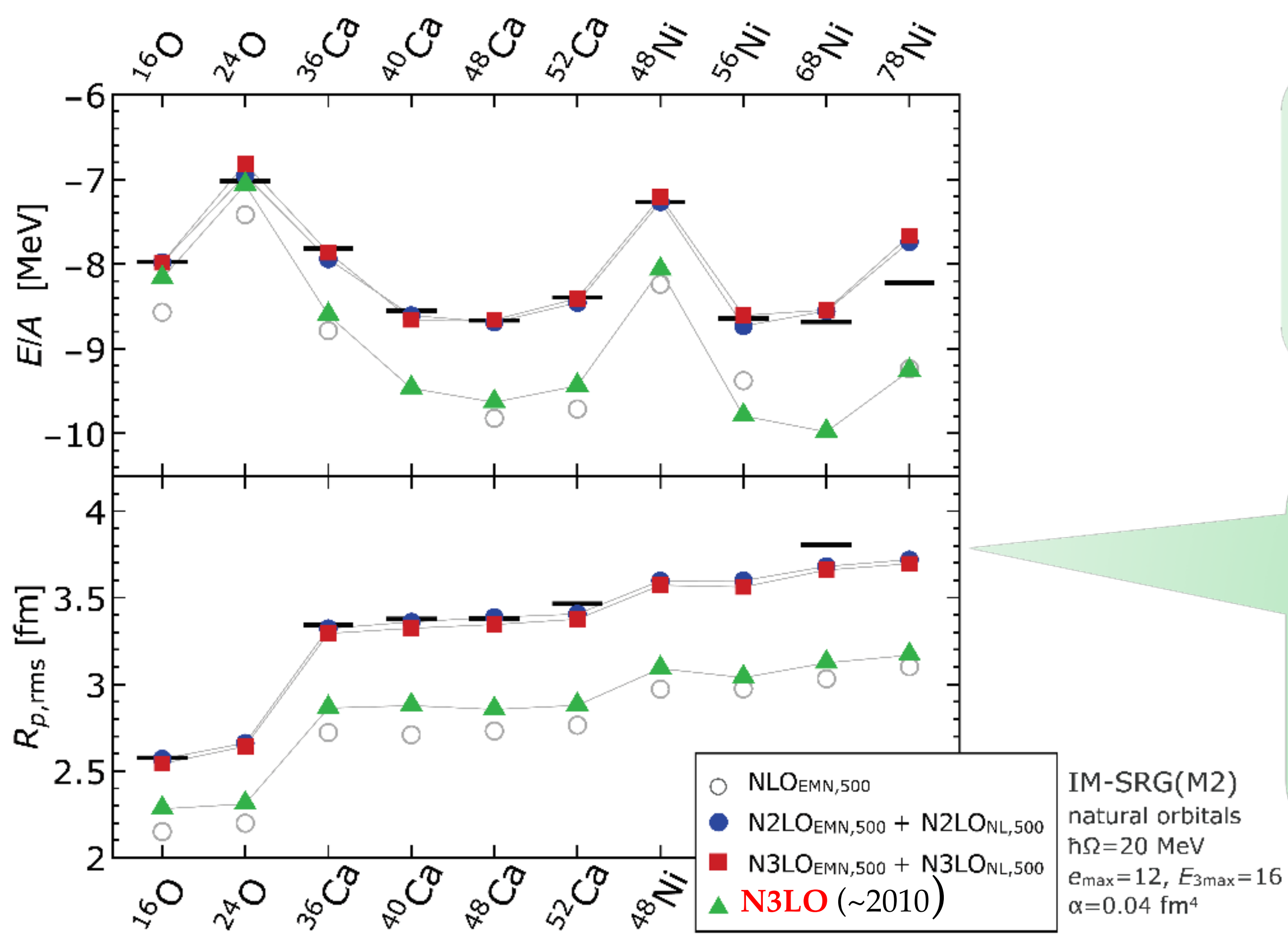




[Somà *et al.* 2019]

◉ Even more recent generation seems to get it all…

[Huther *et al.* 2019]



○ 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

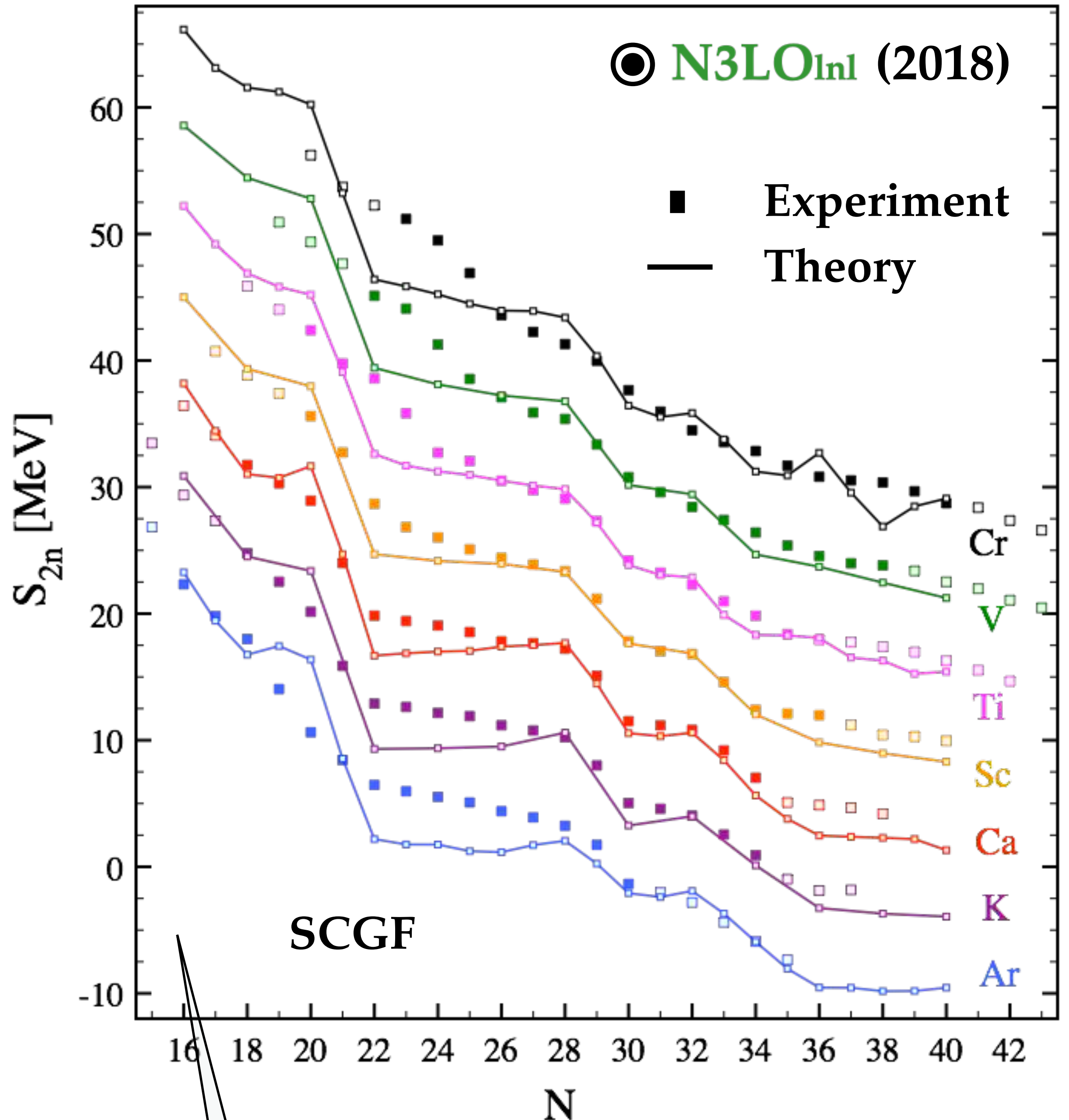
○ Net improvement from NLO to N^{2}LO

○ Stable from N^{2}LO to N^{3}LO

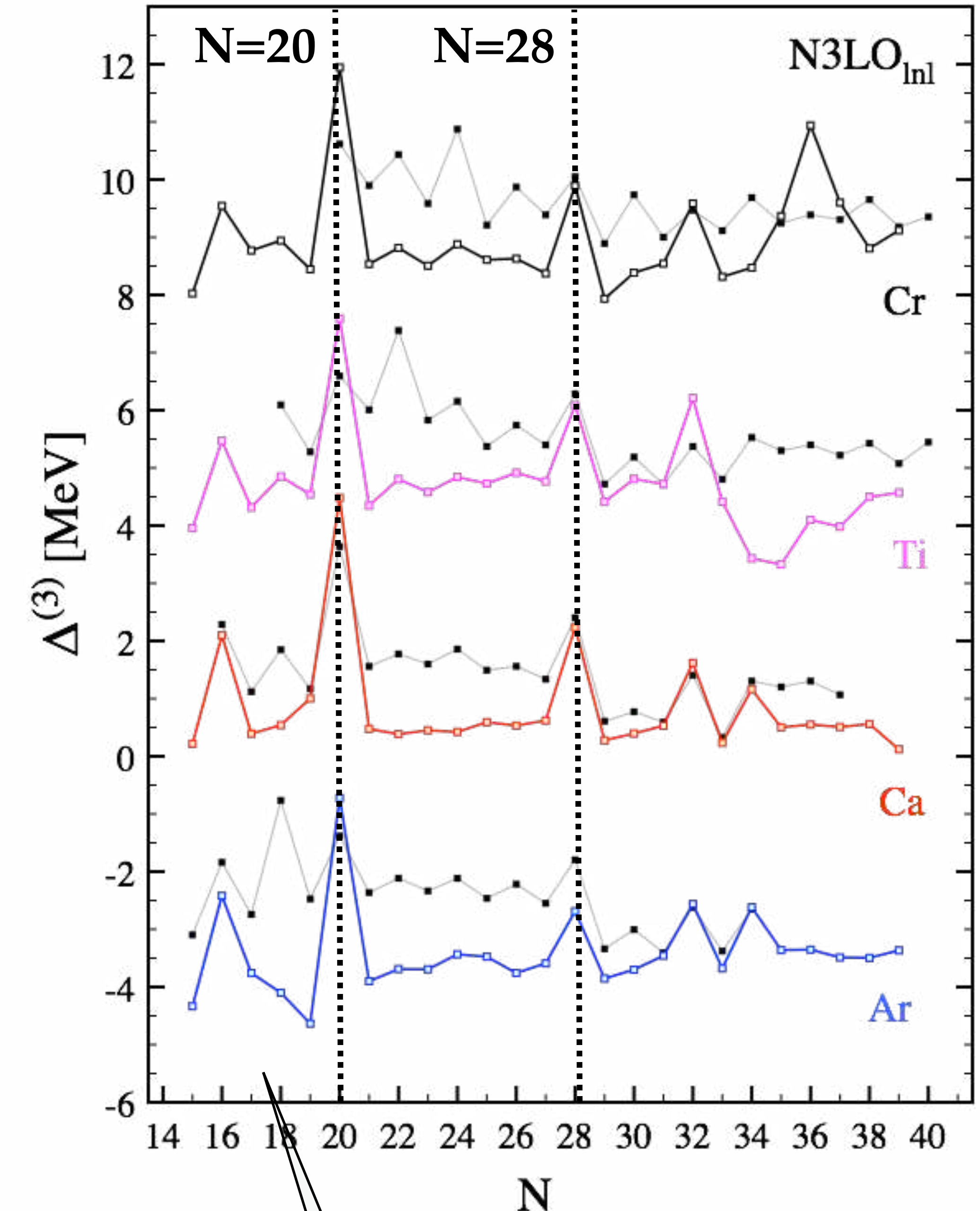
◉ Charge radii provide stringent tests of nuclear interactions via ab initio calculations of mid-mass chains

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

Two-neutron separation energy



Gap size



[Somà *et al.* 2019]

✗ $N = 20$ emerges but overestimated

✓ Good agreement for $N \geq 28$

✓ Main gaps nicely emerge!

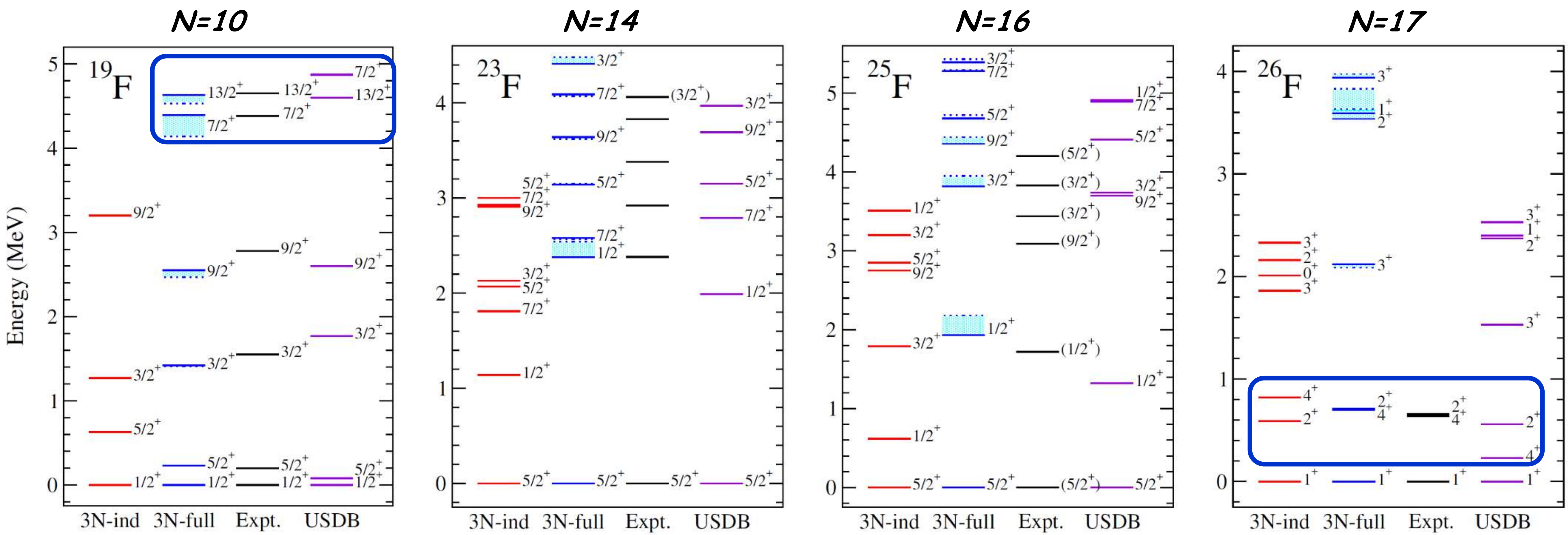
✗ Pairing too weak in $f_{7/2}$

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]

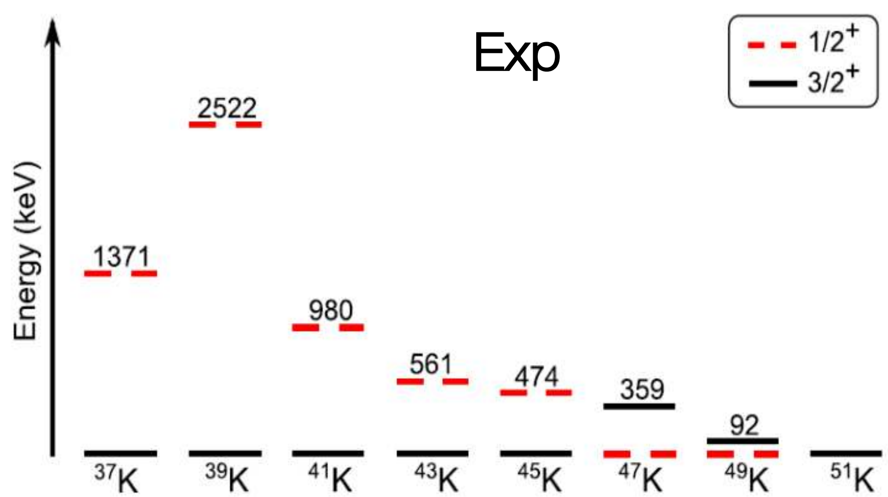
Confrontation with spectroscopic data in sd nuclei can now be based on ab initio scheme!

Spectra of K isotopes

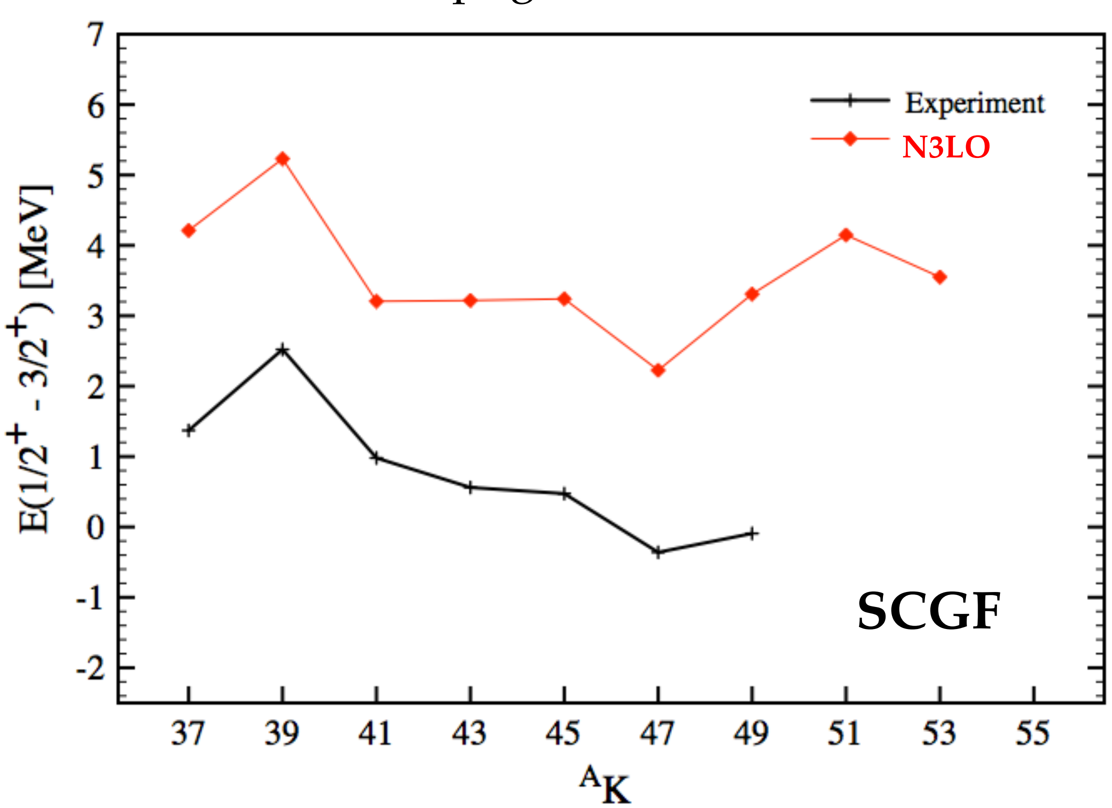
- **K spectra show interesting g.s. spin inversion and re-inversion**

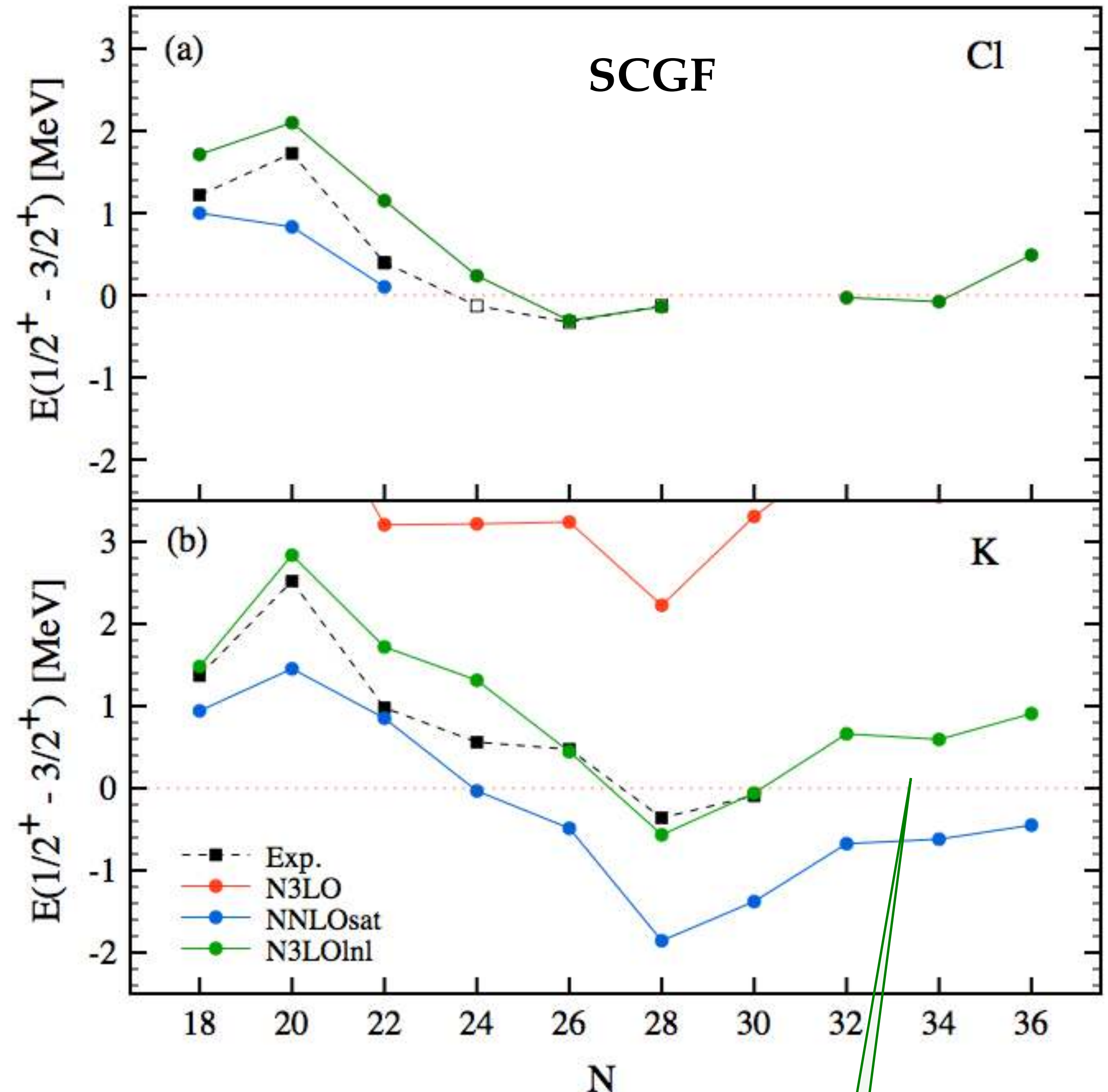
[Somà *et al.* 2019]

Laser spectroscopy COLLAPS @ ISOLDE



[Papuga *et al.* 2013]





Recent experiment confirms N3LOlnl prediction for ^{51}K and ^{53}K

[Sun *et al.* in preparation]

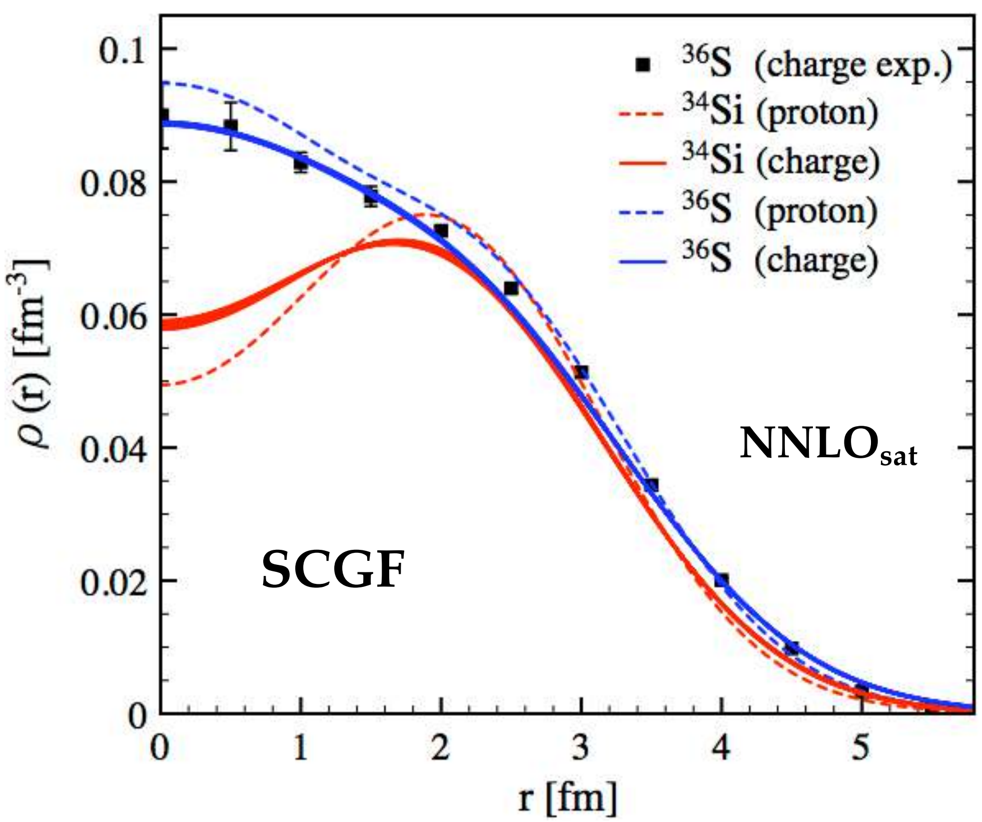
Potential bubble nucleus ^{34}Si

◉ 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]

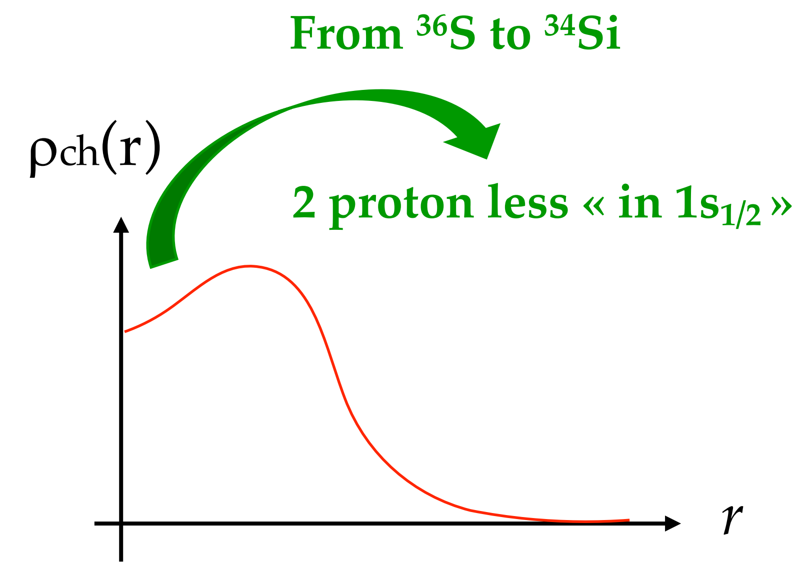


E	ADC(3)	Experiment
^{34}Si	−282.938	−283.427
^{36}S	−305.767	−308.714

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]

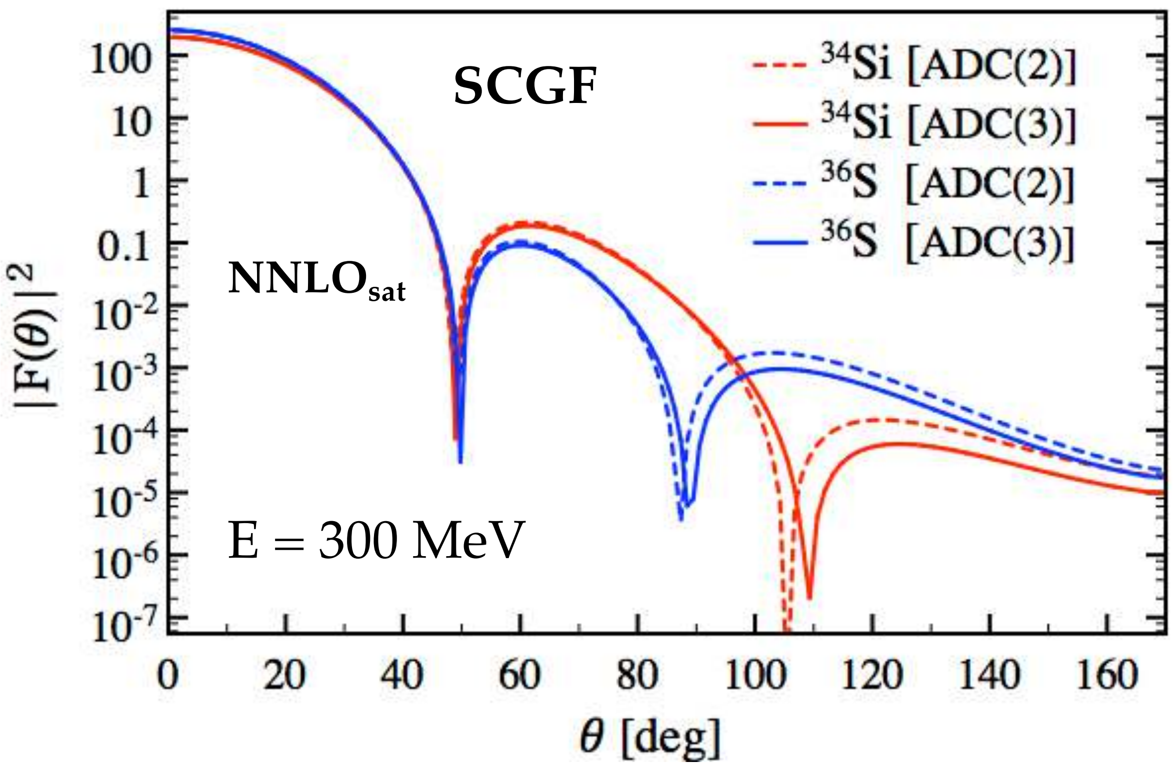
○ **Charge** density of ^{34}Si is predicted to display a **marked depletion in the center**

Charge form factor

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

PWBA

$$F(q) = \int d\vec{r}\rho_{\rm ch}(r)e^{-i\vec{q}\cdot\vec{r}}$$ 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

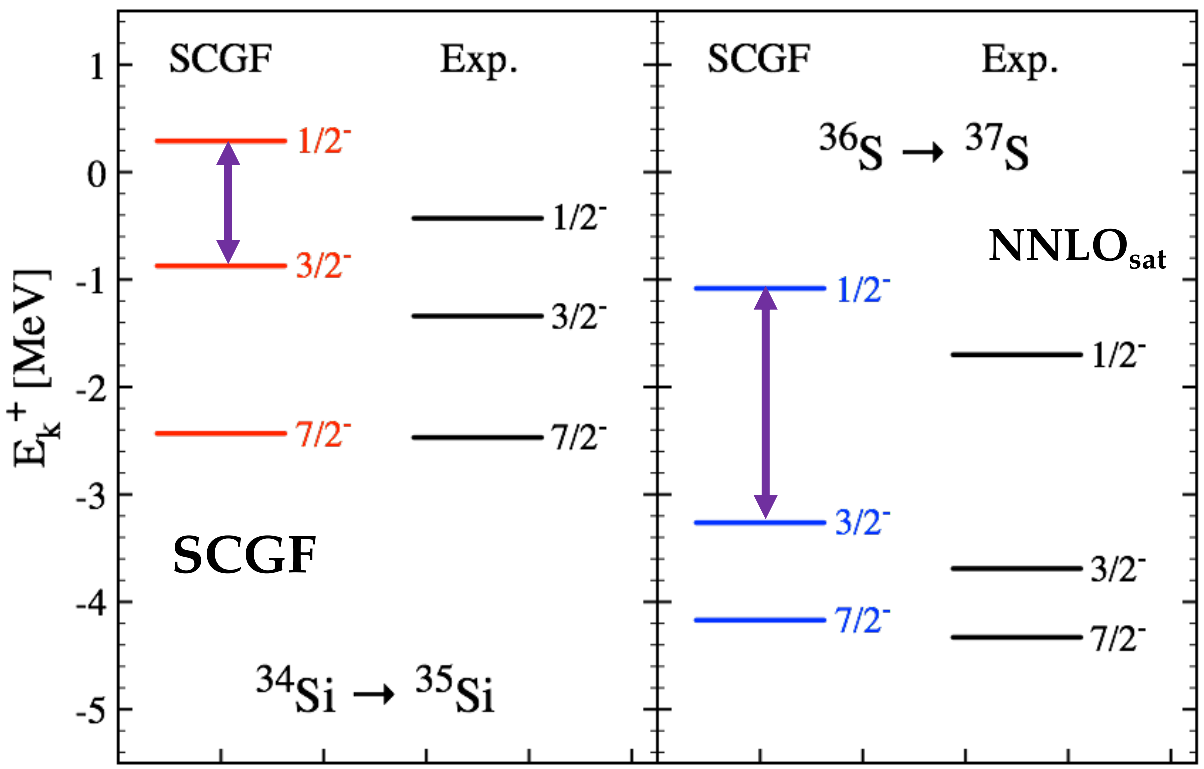
One-neutron addition

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

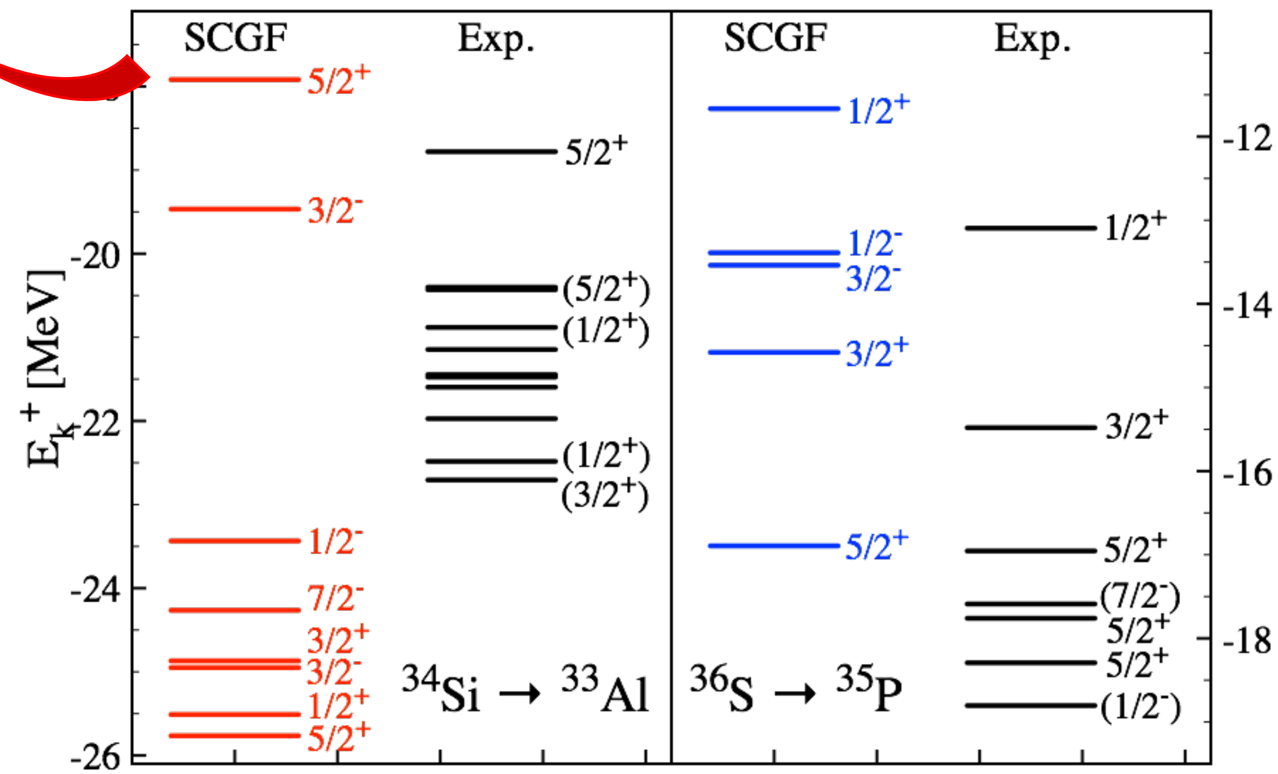
Quadrupole moment [Heylen *et al.* 2016]

One-proton knock-out

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



[Duguet *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**

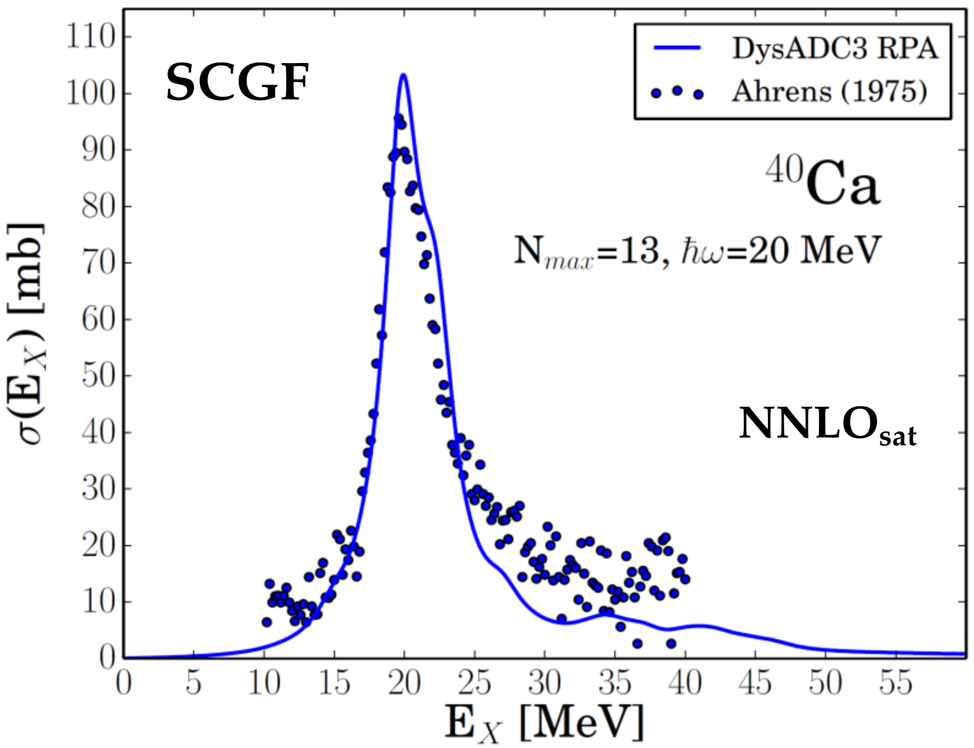
Such a sudden reduction of 50% is unique
Any correlation with the bubble? Yes!

$E_{1/2^-} - E_{3/2^-}$	^{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

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

Electric dipole operator

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

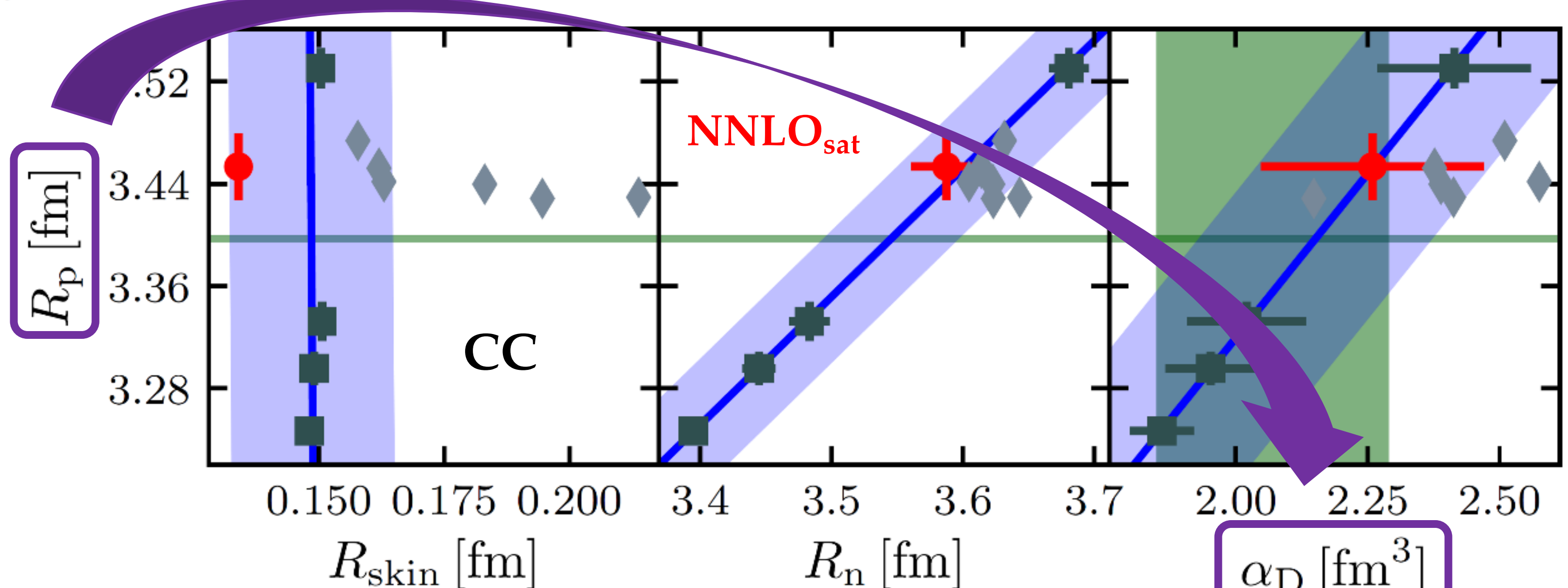
Giant and pygmy resonances accessible up to ^{A}Ni
Many-body correlations crucial for quantitative description

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

Electric dipole polarizability

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

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



[Simonis *et al.* 2019]

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

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

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

- 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

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

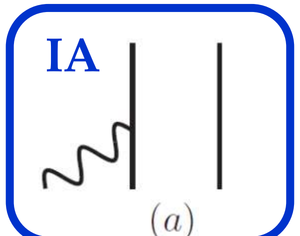
One-body current ↔ NR expansion of covariant single-nucleon current operator
↔ simplified picture that e.m. properties due to free nucleons

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

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

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

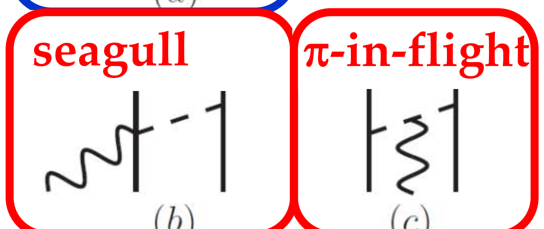
LO $e\,Q^{(-2)}$



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

convection — spin magnetization

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

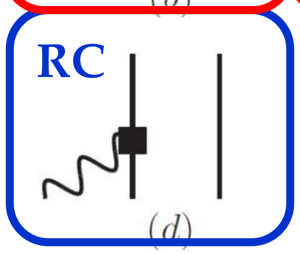


$$\vec{j}^{\,NLO}_{ij}(\vec{k}_i, \vec{k}_j; \vec{q}) = i e \frac{g_A^2}{F_\pi^2}(\vec{\tau}_i \times \vec{\tau}_j)^z \left(\vec{\sigma}_i - \vec{k}_i \frac{\vec{\sigma}_i . \vec{k}_i}{k_i^2 + m_\pi^2}\right)\frac{\vec{\sigma}_j . \vec{k}_j}{k_j^2 + m_\pi^2} + i \rightleftarrows j$$

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

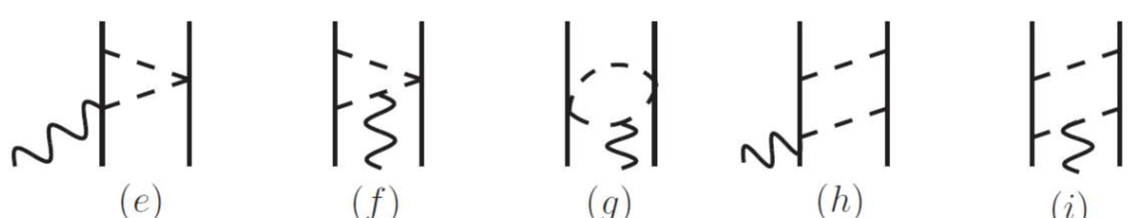
N²LO $e\,Q^{(0)}$



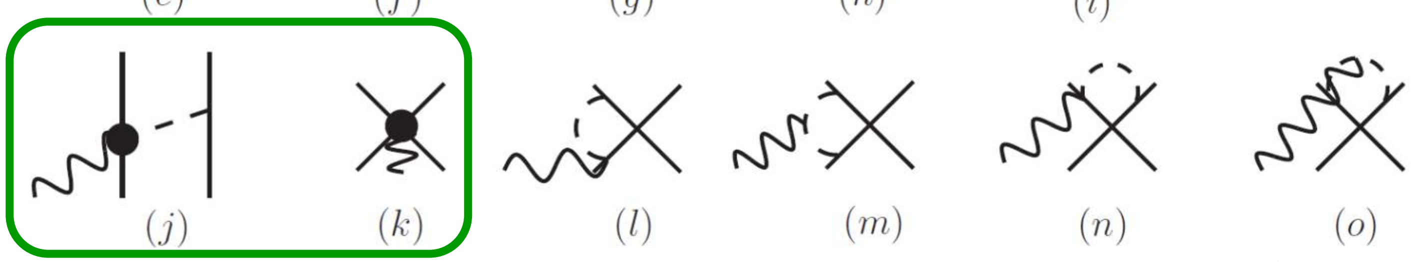
Suppressed by $(Q/m)^2$

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

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

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

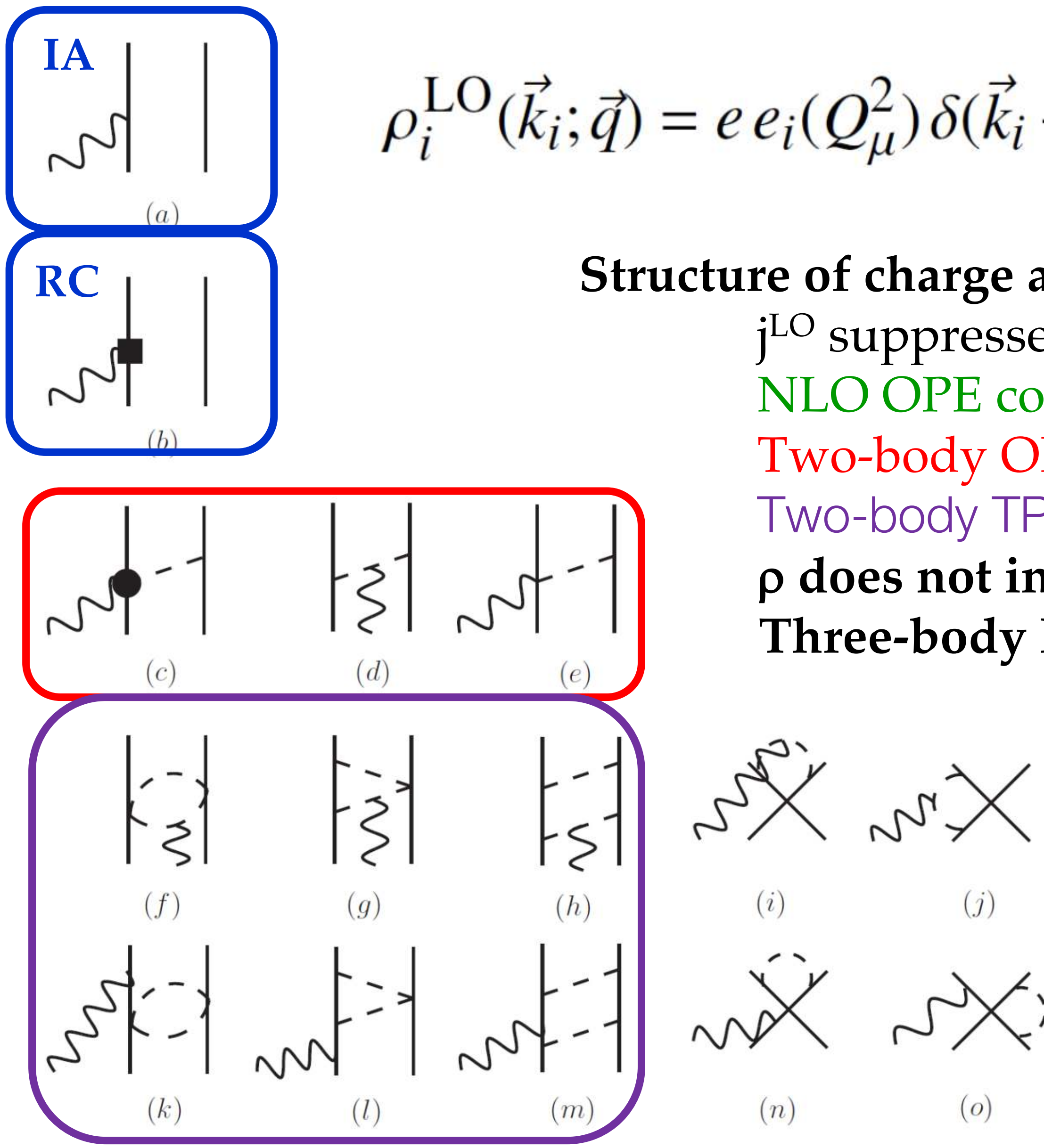
$Q^2_\mu = q^2 - \omega^2$

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

N²LO $e\,Q^{(-1)}$

N³LO $e\,Q^{(0)}$

N⁴LO $e\,Q^{(1)}$



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

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

Nucleon's electric/magnetic form factors

$$e_i(Q^2_\mu) = \frac{G_E^S(Q^2_\mu) + G_E^V(Q^2_\mu)\tau_i^z}{2}$$

$$\mu_i(Q^2_\mu) = \frac{G_M^S(Q^2_\mu) + G_M^V(Q^2_\mu)\tau_i^z}{2}$$

$G_E^S(0) = G_E^V(0) = 1$

$G_M^S(0) = 0.880\mu_N$

$G_M^V(0) = 4.706\mu_N$

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 ← 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 ← **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

$$Q^{\text{IA}} = e \sum_i e_i(0)\, r_i^2\, Y_{20}(\theta_i, \phi_i)$$

○ Static magnetic dipole operator

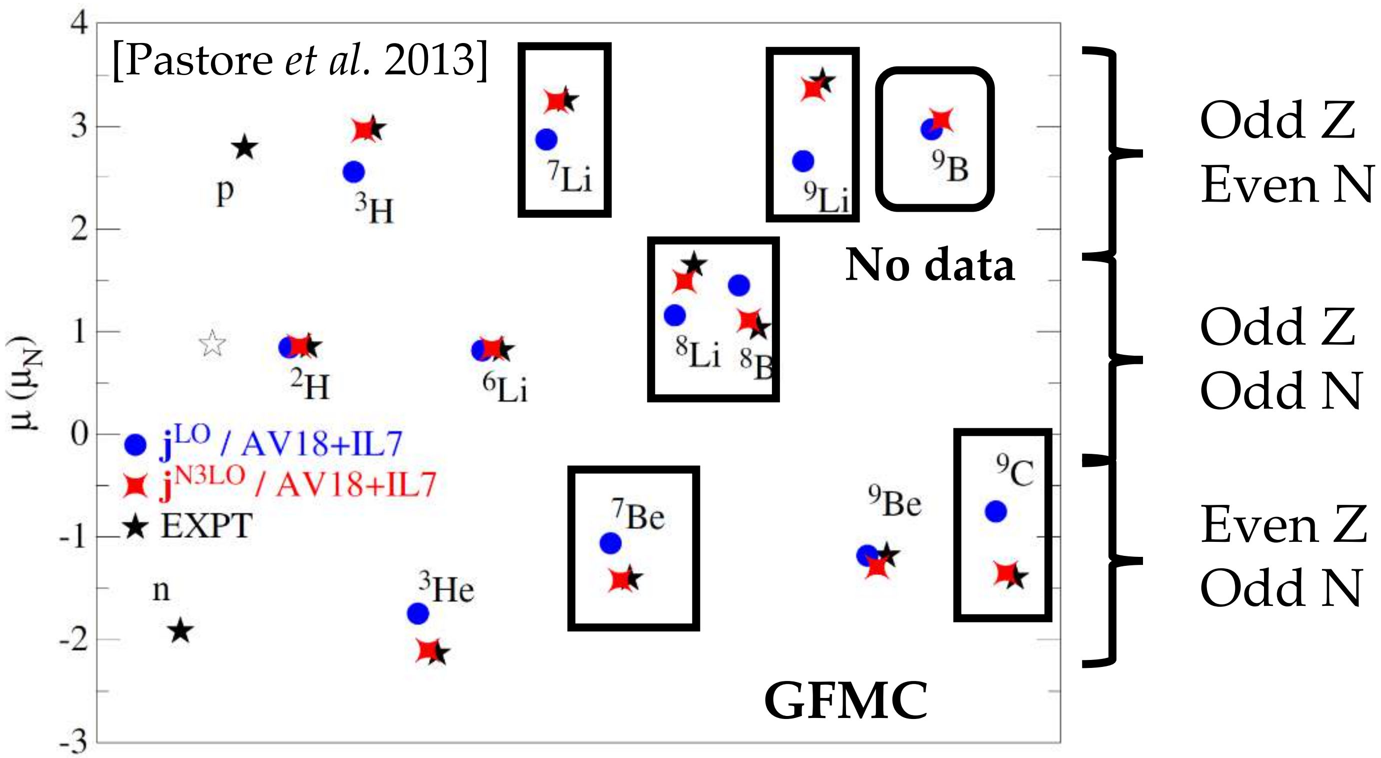
$$\mu^{\text{IA}} = \sum_i e_i(0)\, \vec{L}_i + \mu_i(0)\, \vec{\sigma}_i$$

Contents

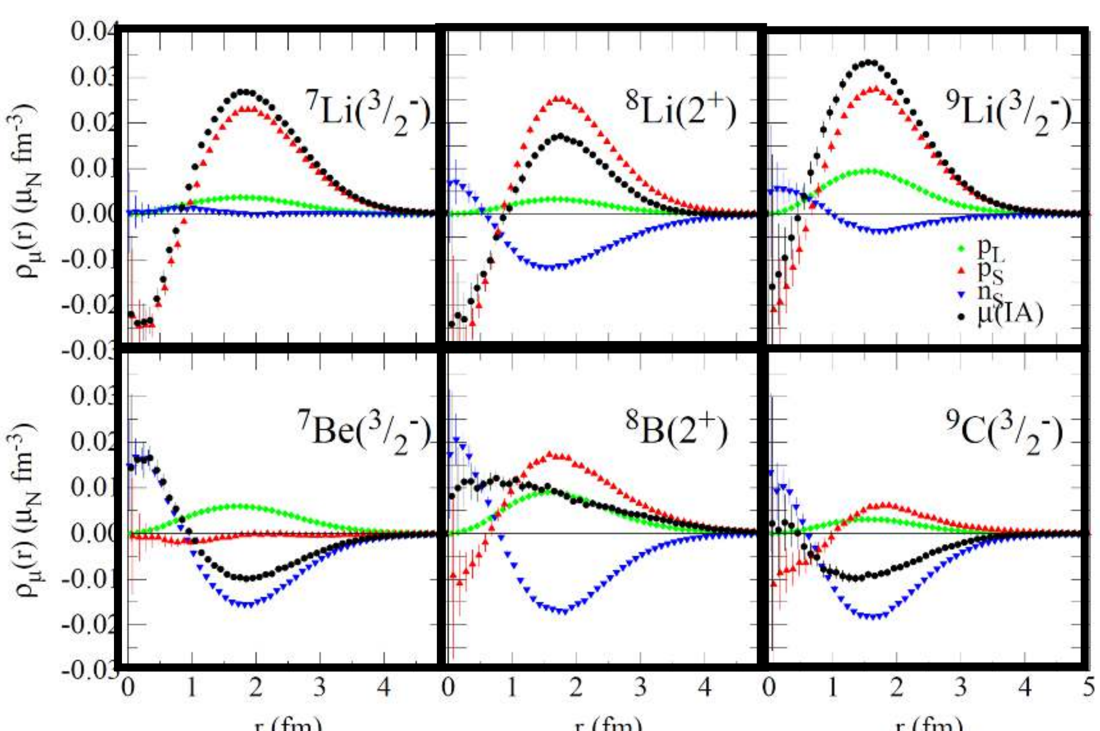
- Introduction of the nuclear Ab initio nuclear quantum many-body problem
  - Definition and recent progress
  - Examples of recent applications
  - Some challenges and on-going developments
- Ab initio nuclear many-body problem and observables accessible via laser spectroscopy
  - Direct observables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

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**

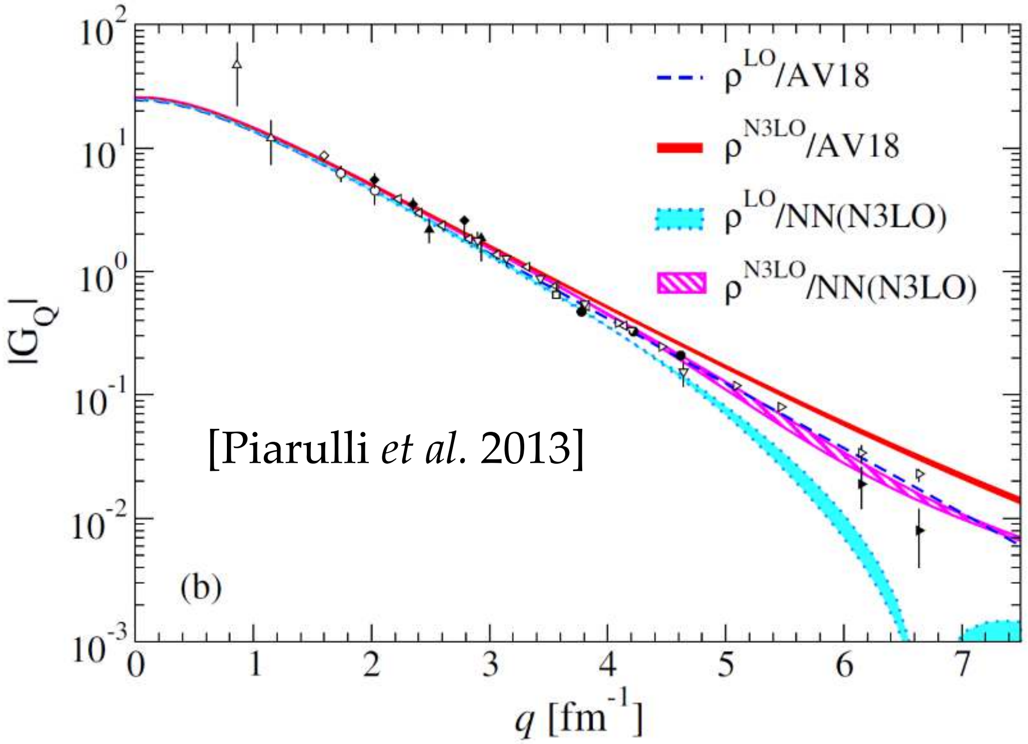
- ○ Excellent account of data
- ○ Dominated by one-body (IA)
- ○**Two-body MEC up to 40%**
- ○ MEC (almost) always improve

◉ **Decomposition of one-body IA**

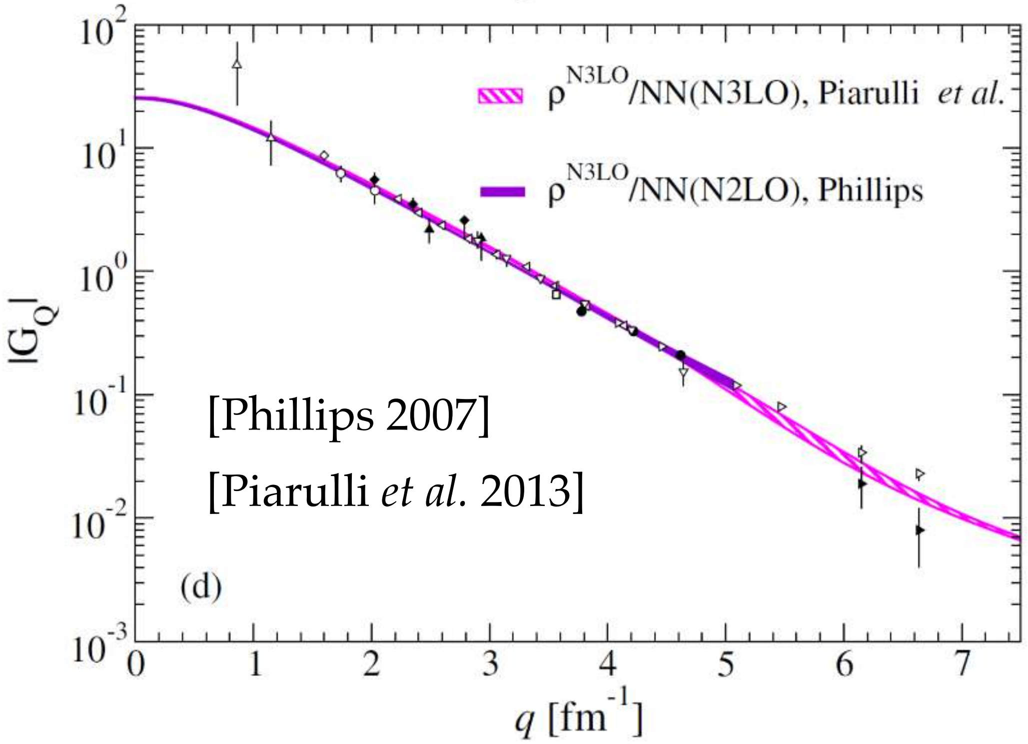
- ○ Proton's convection small vs spin magnetization
- ○ **Driven by valence nucleon in odd-even**
- ○ **Driven by n-p or 3He-p cluster in odd-odd**

Elastic form factors in s and p shell nuclei

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



[Piarulli *et al.* 2013]



[Phillips 2007]

[Piarulli *et al.* 2013]

◉ **Ex: Quadrupole electric form factor in ^2H**

○ Hybrid and (semi-consistent) χ-EFT calculations

○ **Charge operator at LO (IA) and N^{3}LO**

○ 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^{3}LO MEC excellent up to q ~ 8 fm^{-1}**

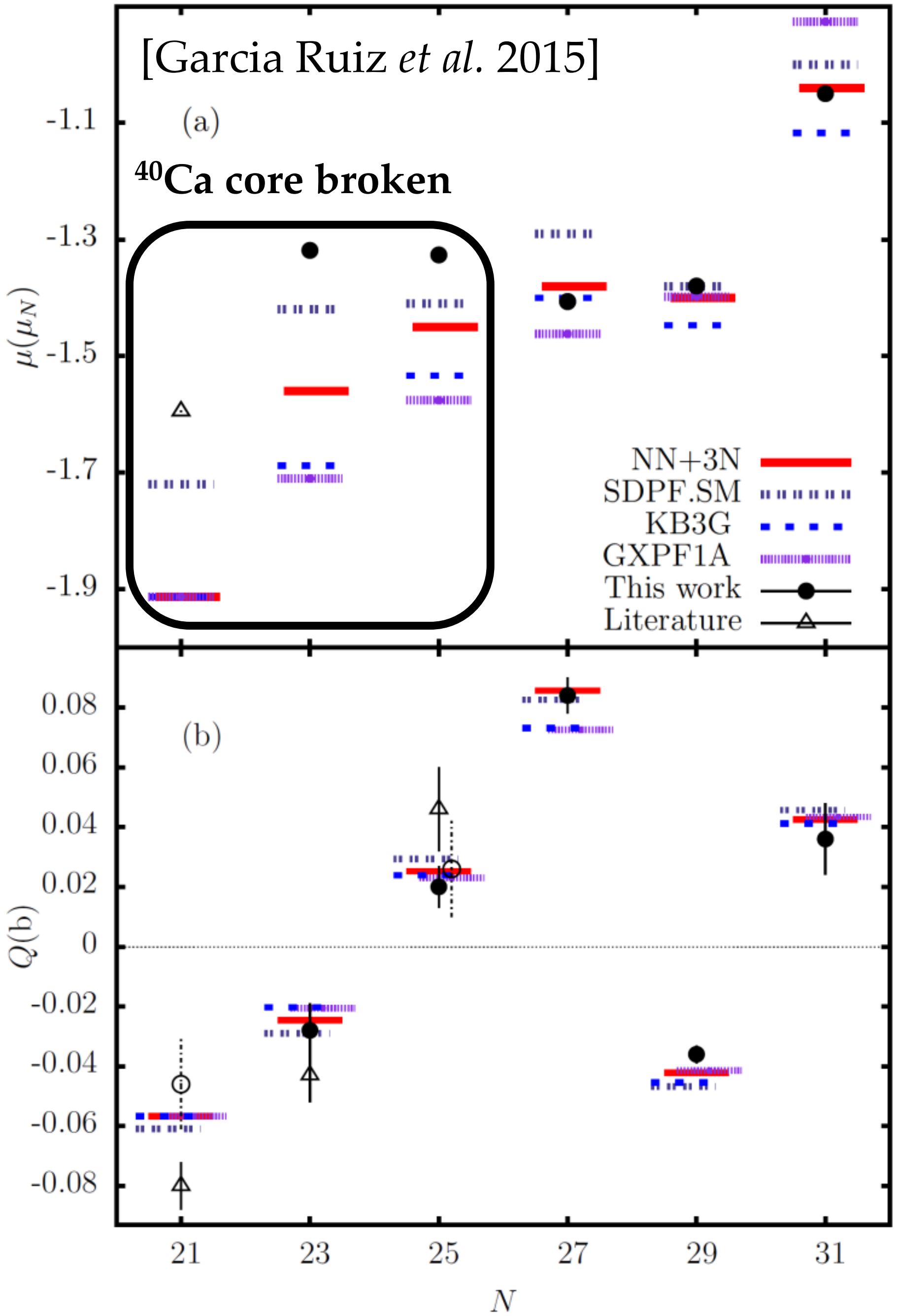
Contents

- 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

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

Huge diversity of nuclear phenomena

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

Several scales at play:

p & n momenta ~ $\mathbf{10^8}$ eV

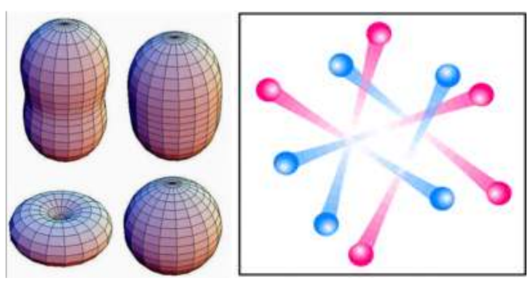
Separation energies ~ $\mathbf{10^7}$ eV

Vibrational excitations~ $\mathbf{10^6}$ eV

Rotational excitations ~ $\mathbf{10^4}$ eV

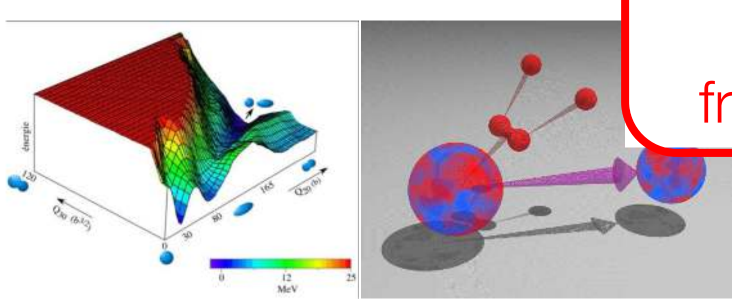
Ground state

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



Radioactive decays

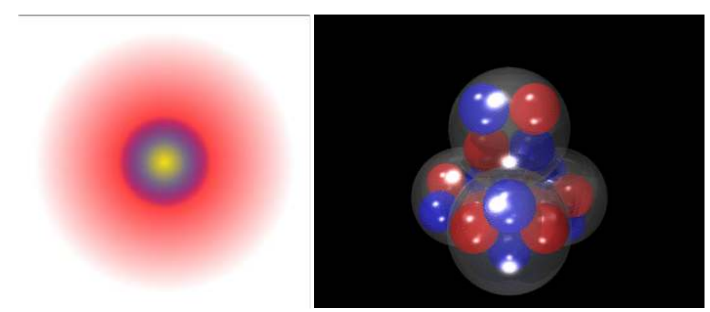
β, 2β, $0\nu2\beta$, α, p, 2p, ($\neq$



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

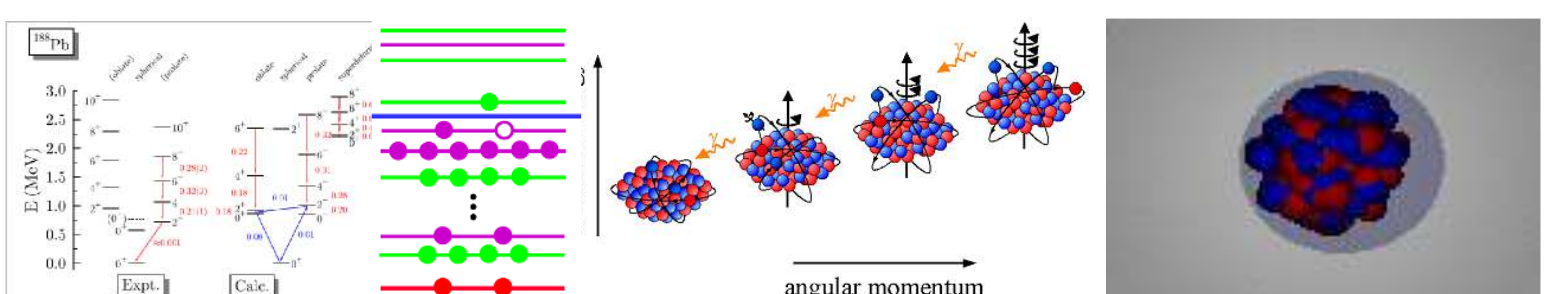
Exotic structures

Clusters, halos, …



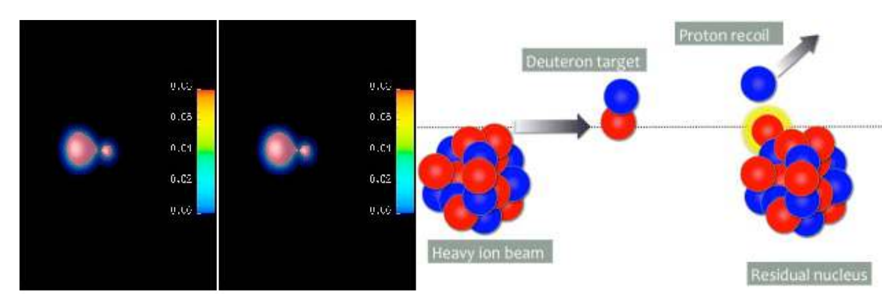
Spectroscopy

Excitation modes



Reaction processes

Fusion, transfer, knockout, …



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

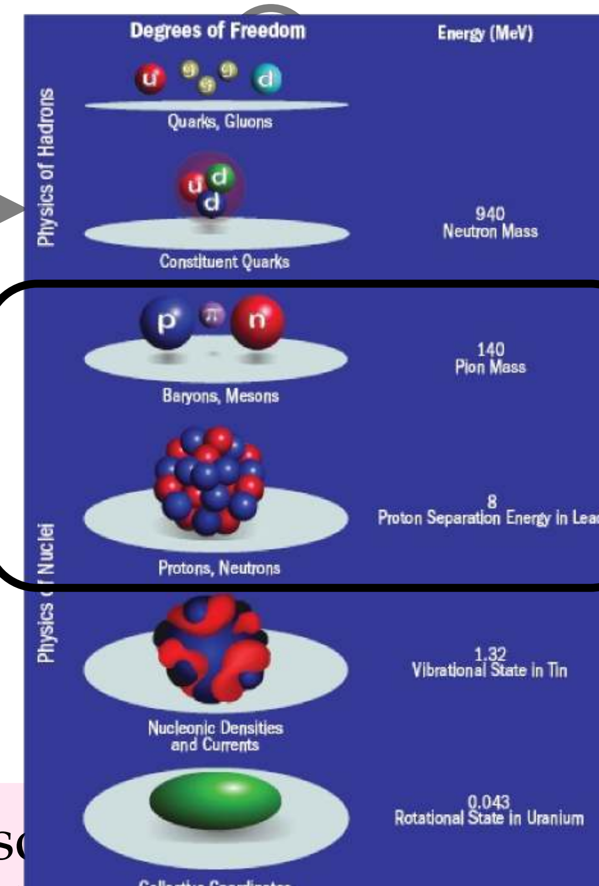
Definition

- *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*



3 *QCD* *Data*

$B(E\lambda), \ldots$?

"Ab initio"

tion *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 so... 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?

Ab initio vs effective approach

***Ab initio* (= "from scratch") many-body scheme**

$$H|\Psi^A_k\rangle = E^A_k|\Psi^A_k\rangle$$

A-body Hamiltonian

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

A-body wave-function

5 variables x A nucleons

Effective approach = reduce the dimensionality of active many-body Hilbert space

Two options

- Reduce active **one**-body Hilbert space → Ex: Interacting shell model
- Restrict directly **many**-body Hilbert space → Ex: Energy density functional

$$H^{eff}|\Phi^{eff}_k\rangle = E^A_k|\Phi^{eff}_k\rangle$$

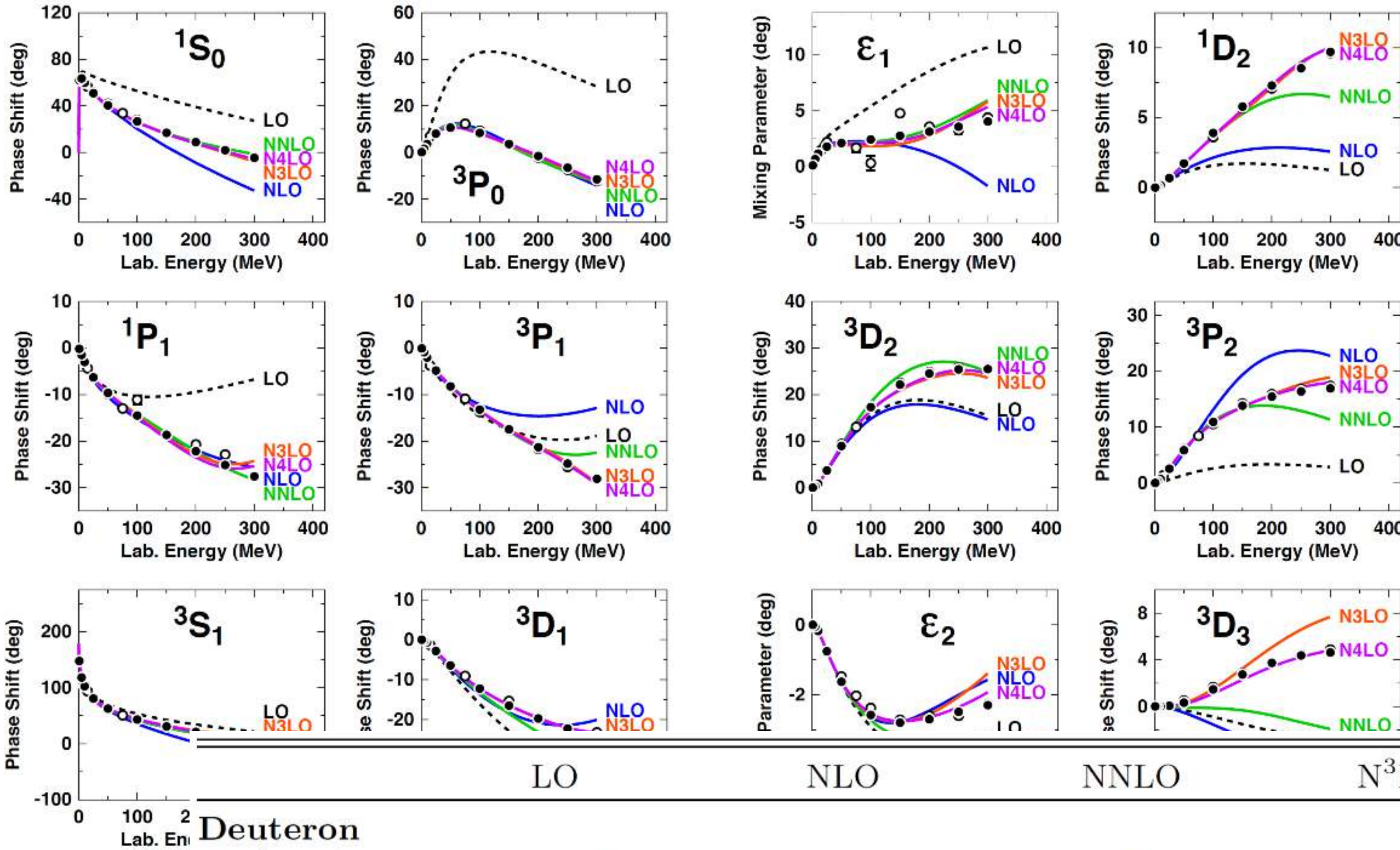
Must in principle exactly compensate… no gain

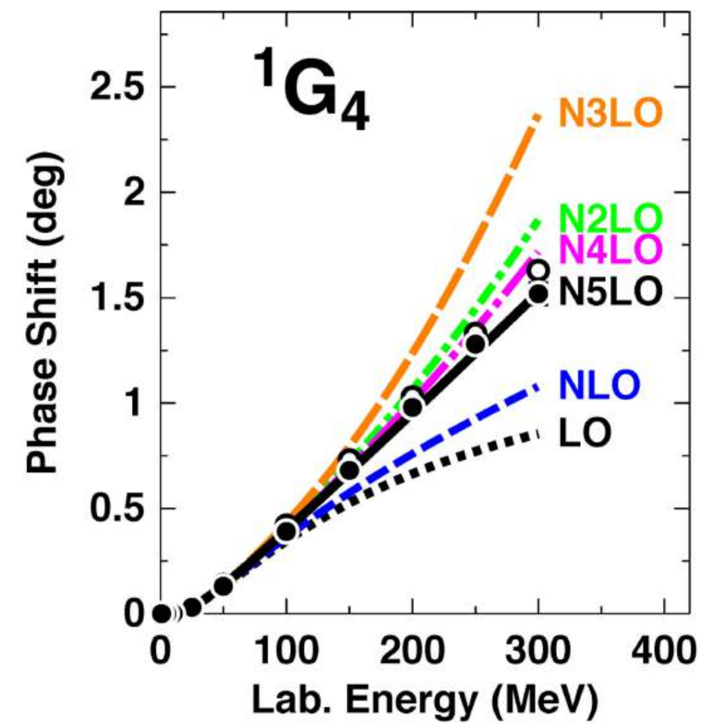
Build approximations… so far done empirically

Matter of choice

- ◉ Which properties we aim at and which level of accuracy are we seeking?
- ◉ Applicability throughout the nuclear chart? → Universal/global vs local description
- ◉ Wish to connect to underlying theory of strong force or wish to focus on describing data?
- ◉ Predictive power? → Estimate of theoretical error

Chiral effective field theory = basic considerations





	LO	NLO	NNLO	N^{3}LO	N^{4}LO	Empirical[a]
Deuteron						
B_d (MeV)	2.224575	2.224575	2.224575	2.224575	2.224575	2.224575(9)
A_S (fm$^{-1/2}$)	0.8526	0.8828	0.8844	0.8853	0.8852	0.8846(9)
η	0.0302	0.0262	0.0257	0.0257	0.0258	0.0256(4)
$r_{\rm str}$ (fm)	1.911	1.971	1.968	1.970	1.973	1.97507(78)
Q (fm^2)	0.310	0.273	0.273	0.271	0.273	0.2859(3)
P_D (%)	7.29	3.40	4.49	4.15	4.10	—
Triton						
B_t (MeV)	11.09	8.31	8.21	8.09	8.08	8.48

:hiral EFT.

						N^{4}LO
						1.09
						1.12
						1.21
neutron-proton						
0–100	1180	114	7.2	1.38	0.93	0.94
0–190	1697	96	23.1	2.29	1.10	1.06
0–290	2721	94	36.7	5.28	1.27	1.10
pp* plus *np						
0–100	1975	283	11.9	1.74	1.03	1.00
0–190	2903	235	31.6	3.27	1.35	1.08
0–290	4853	206	51.5	6.30	1.63	1.15

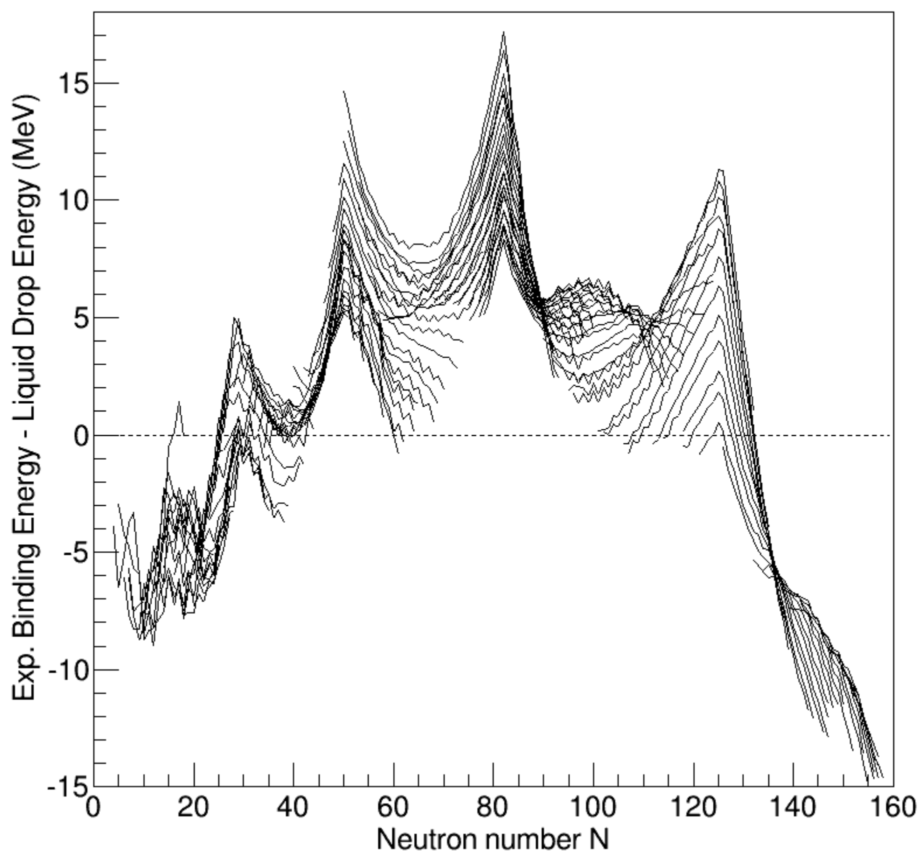
Similarities and differences with quantum chemistry

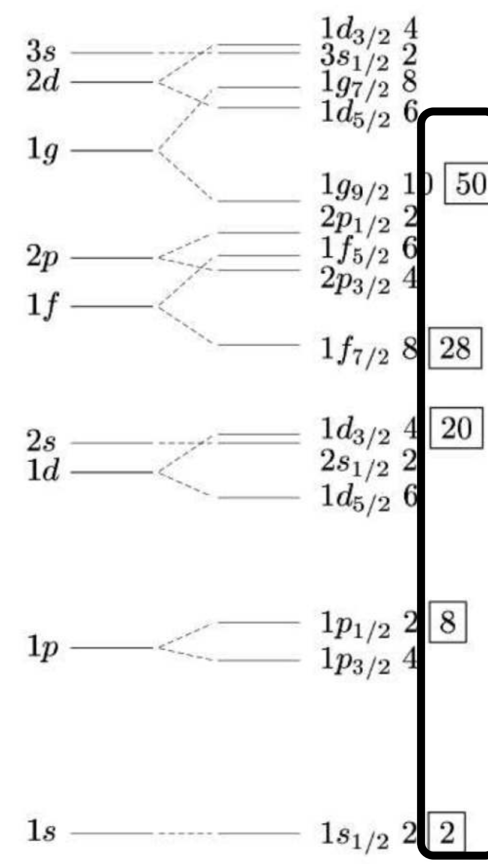
Zeroth-order model
↕
Filling of neutron/proton shells

Major closed shells
↕
Magic numbers

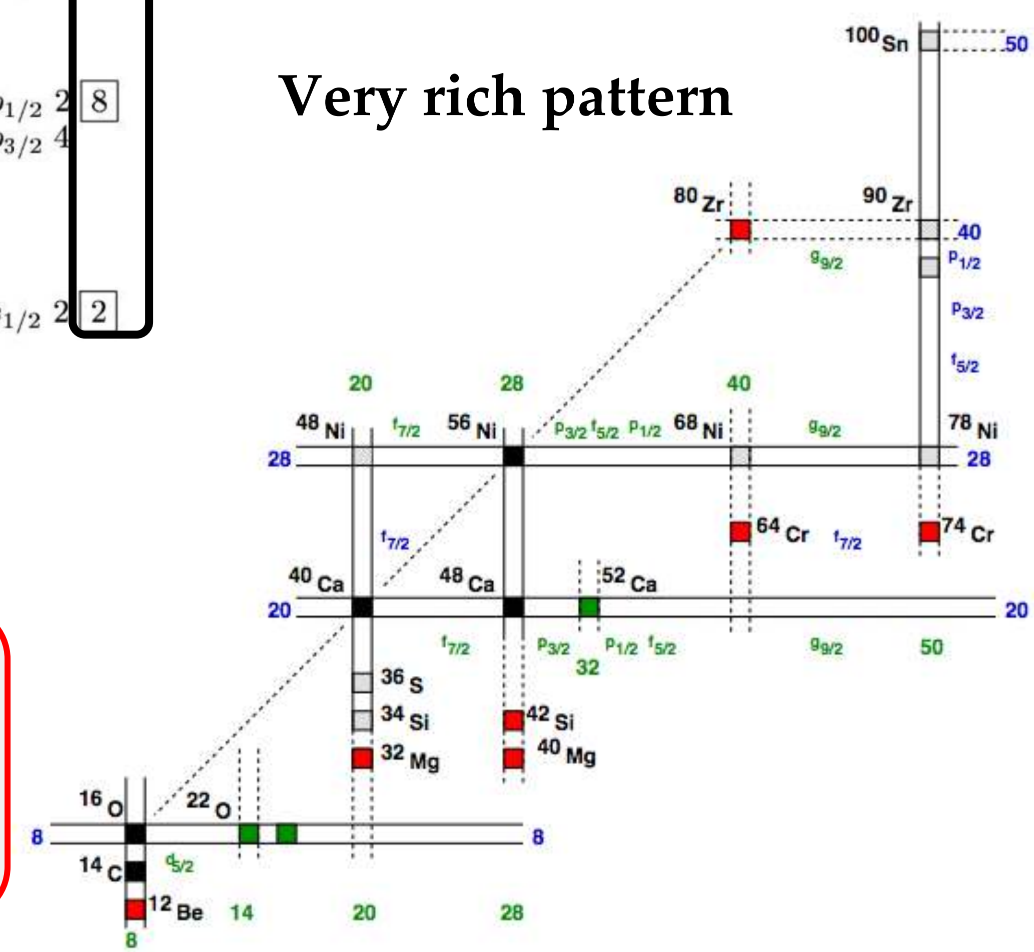
+
Minor closed shells
+
Modification with N-Z
+
Many-body correlations
=

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





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?

Hamiltonian

Nuclear Hamiltonian

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

Genuine 3N interaction / six-legs vertex

Particle number

$$A \equiv \sum_p c_p^\dagger c_p$$

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 (λ)

↓

Controls the average particle number in the system

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

$$H \equiv \Lambda^{00}$$
$$+ \frac{1}{1!1!} \sum_{l_1 l_2} \Lambda^{11}_{l_1 l_2} : c_{l_1}^\dagger c_{l_2} :$$
$$+ \frac{1}{2!2!} \sum_{l_1 l_2 l_3 l_4} \Lambda^{22}_{l_1 l_2 l_3 l_4} : c_{l_1}^\dagger c_{l_2}^\dagger c_{l_4} c_{l_3} :$$
$$+ \frac{1}{3!3!} \sum_{l_1 l_2 l_3 l_4 l_5 l_6} \Lambda^{33}_{l_1 l_2 l_3 l_4 l_5 l_6} : c_{l_1}^\dagger c_{l_2}^\dagger c_{l_3}^\dagger c_{l_6} c_{l_5} c_{l_4} :$$

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

$$\beta_k = \sum_p U^*_{pk} c_p + V^*_{pk} c^\dagger_p \qquad |\Phi\rangle \equiv C \prod_k \beta_k |0\rangle \qquad A|\Phi\rangle \neq \mathrm{A}|\Phi\rangle$$

$$\beta^\dagger_k = \sum_p U_{pk} c^\dagger_p + V_{pk} c_p \qquad \beta_k |\Phi\rangle = 0 \quad \forall k$$

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

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

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

H^{ij} matrix elements function of

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

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

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

6-qp operators

Similarly for A and Ω

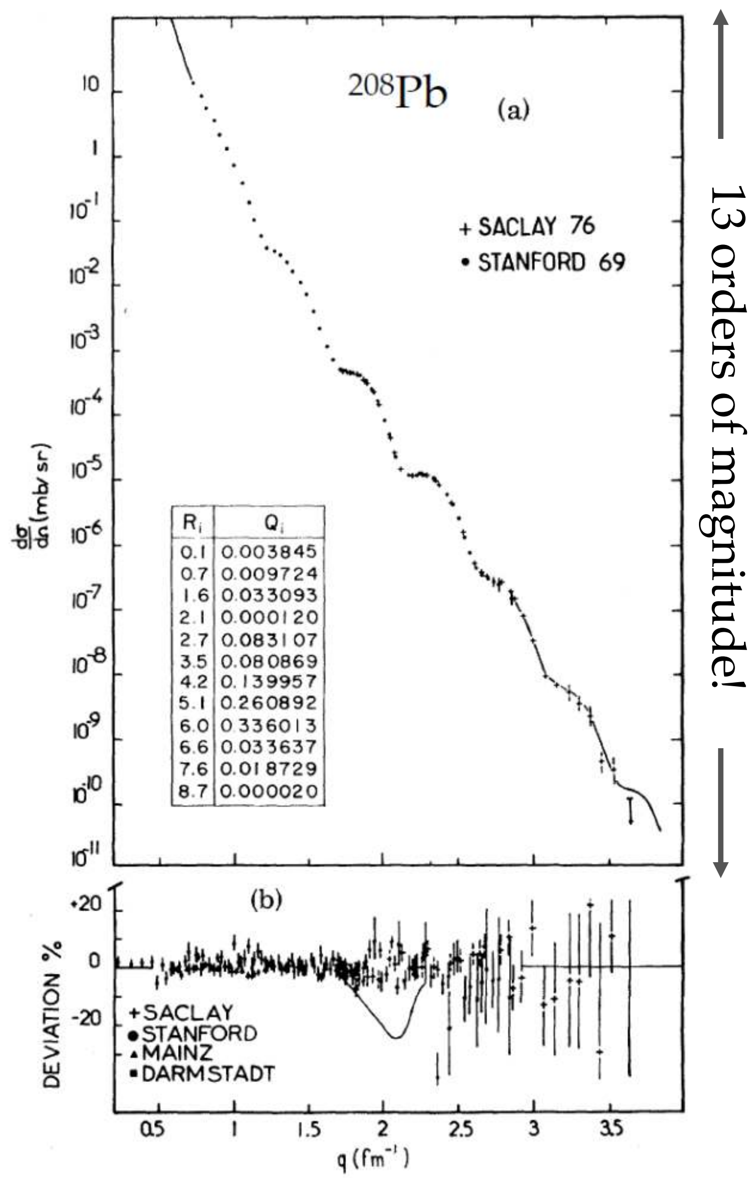
Six-index tensors
Too expensive to handle

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]

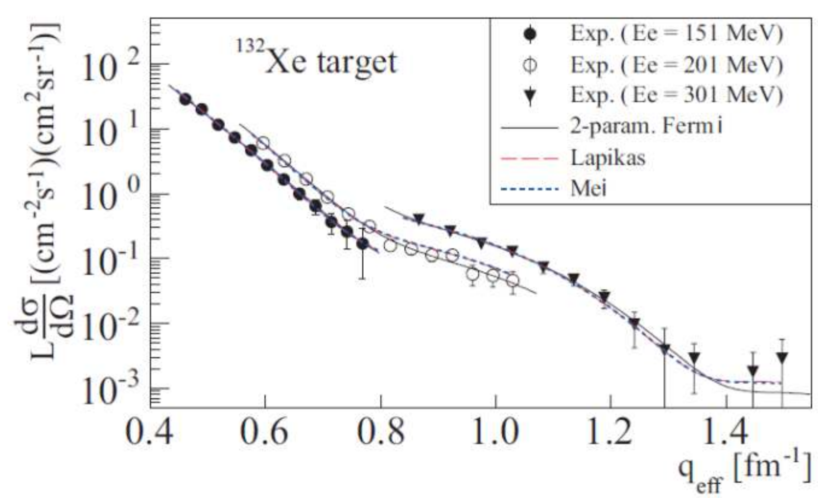
Electron scattering off nuclei

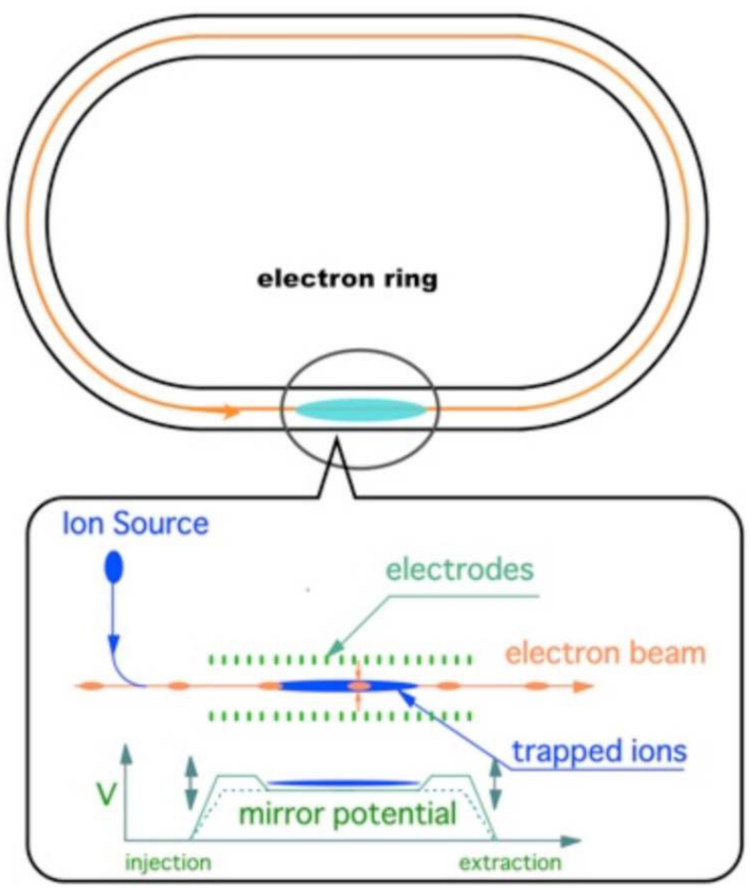
- ◉ Electrons constitute an optimal probe to study atomic nuclei
  - ○ Point-like → excellent spatial resolution
  - ○ EM weak and theoretically well constrained
- ◉ Accélérateur Linéaire @ Saclay (ALS)
  - ○ Electron accelerator (1969-1990)
  - ○ Refined data on tens of stable nuclei



[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

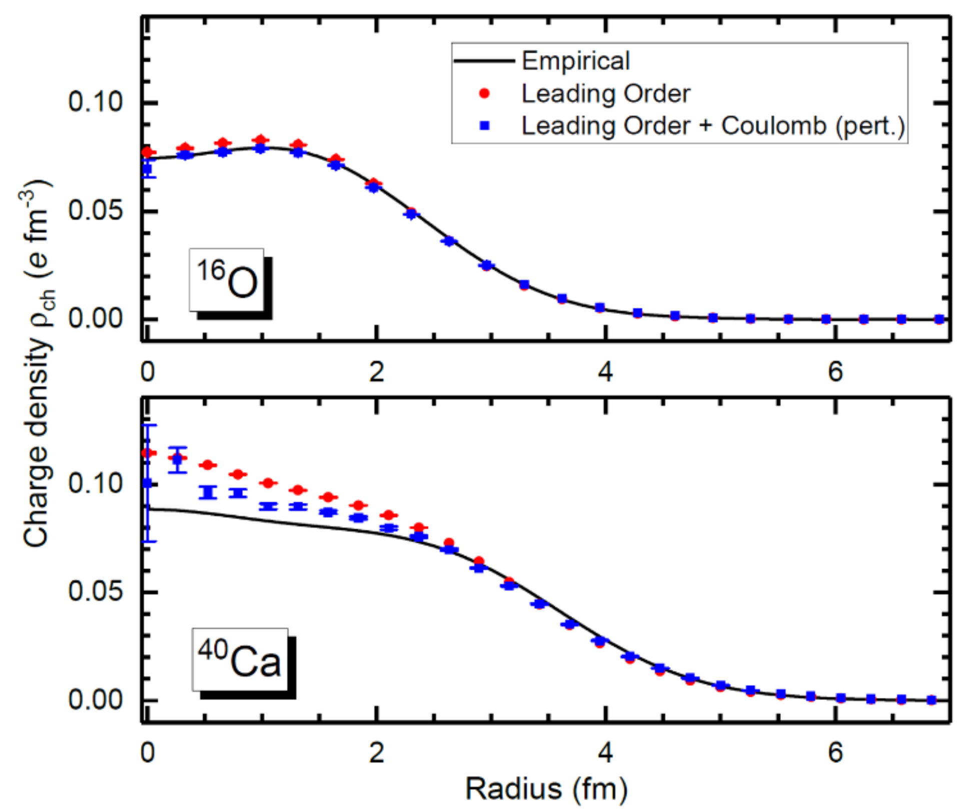
C_2	2N
C_3	3N
S_L	Local part
S_{NL}	Non-local part

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

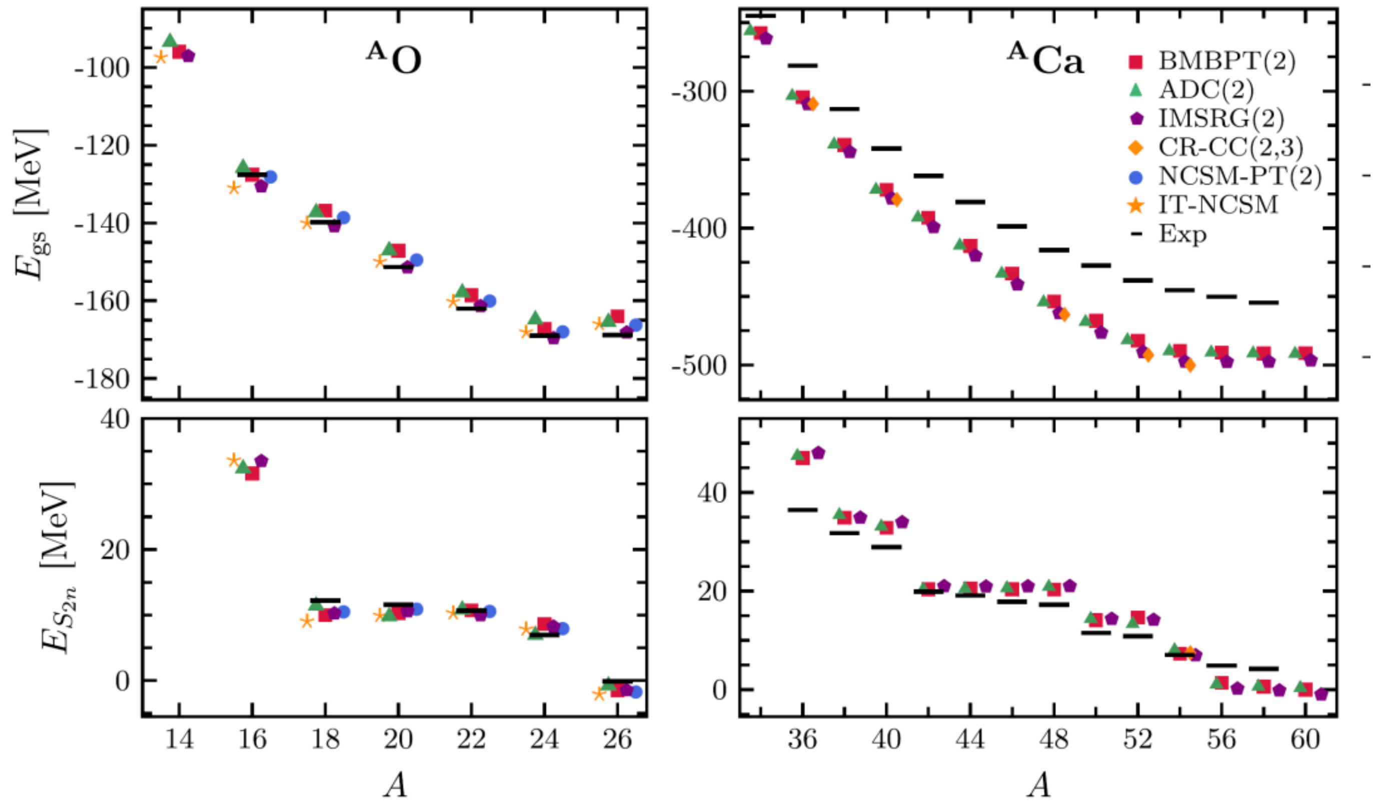
◉ No real free lunch but still look for best compromise
✓ Versatility (nuclei and / or states / observables)
✓ Accuracy
✓ CPU cost

[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