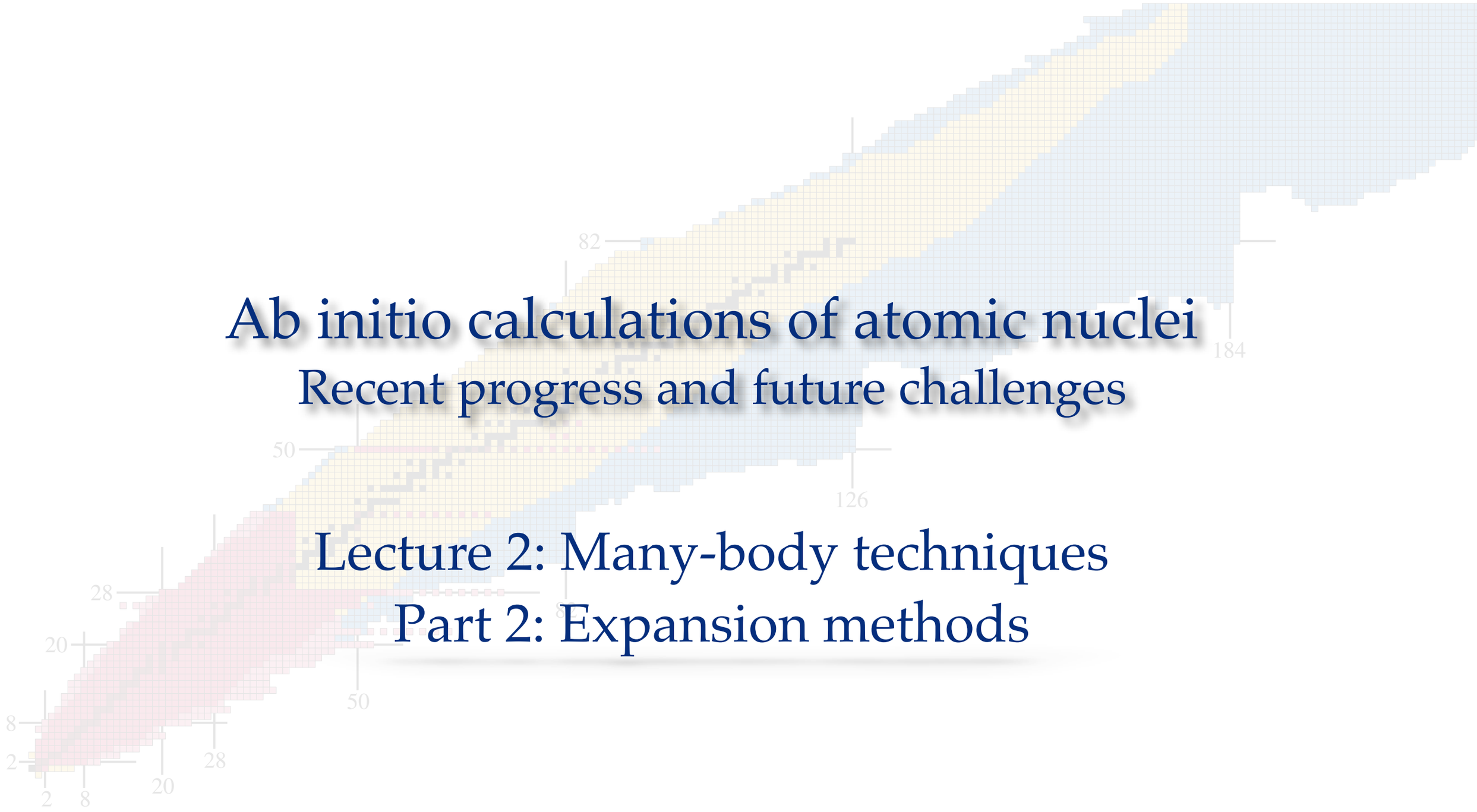

Ab initio calculations of atomic nuclei

Recent progress and future challenges

Lecture 2: Many-body techniques

Part 2: Expansion methods

Università di Padova
7-10 June 2021

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CEA Saclay

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Correlation expansion methods: the idea

- The goal is always to solve $H|\Psi_k^A\rangle = E_k^A|\Psi_k^A\rangle$
- Idea: write the exact ground-state wave function as

$$|\Psi_0^A\rangle = \Omega_0|\phi_0\rangle$$

wave operator / correlation operator — **reference state**

➪ Expansion in terms of **particle-hole excitations**

then **expand** and **truncate** Ω_0

➪ Before truncation, the expansion is **exact**

➪ After truncation, **cost reduced** from $N!$ to N^α with $\alpha \geq 4$

- **Reference state**
  - Must be simple enough (such that it can be computed easily and exactly)
  - Must be rich enough (such that it is a suitable starting point for the expansion)
  - Obtained by

1) Splitting $H = H_0 + H_1$ 2) Solving for H_0 (one-body operator) $H_0|\phi_k\rangle = \epsilon_k|\phi_k\rangle$

Concept of mean field

- **Slater determinant** as reference state
  - One-body potential: $H_0 = \sum_{i=1}^{A} h_0(i) \quad \rightarrow \quad H_0|\phi_k\rangle = \epsilon_k|\phi_k\rangle$ ⇒ $h_0|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle \quad \forall i$

    A-body problem A one-body problems
  - Build Slater $|\phi_0\rangle = \prod_{i=1}^{A} a^\dagger_{\alpha_i}|0\rangle$
  - Independent particles: nucleons move inside a (one-body) potential well or ***mean field***

- **Does an independent-particle picture make any sense at all?**
  - Inter-particle distance in nuclei ~ 2 fm
  - Range of nuclear interaction ~ 2 fm

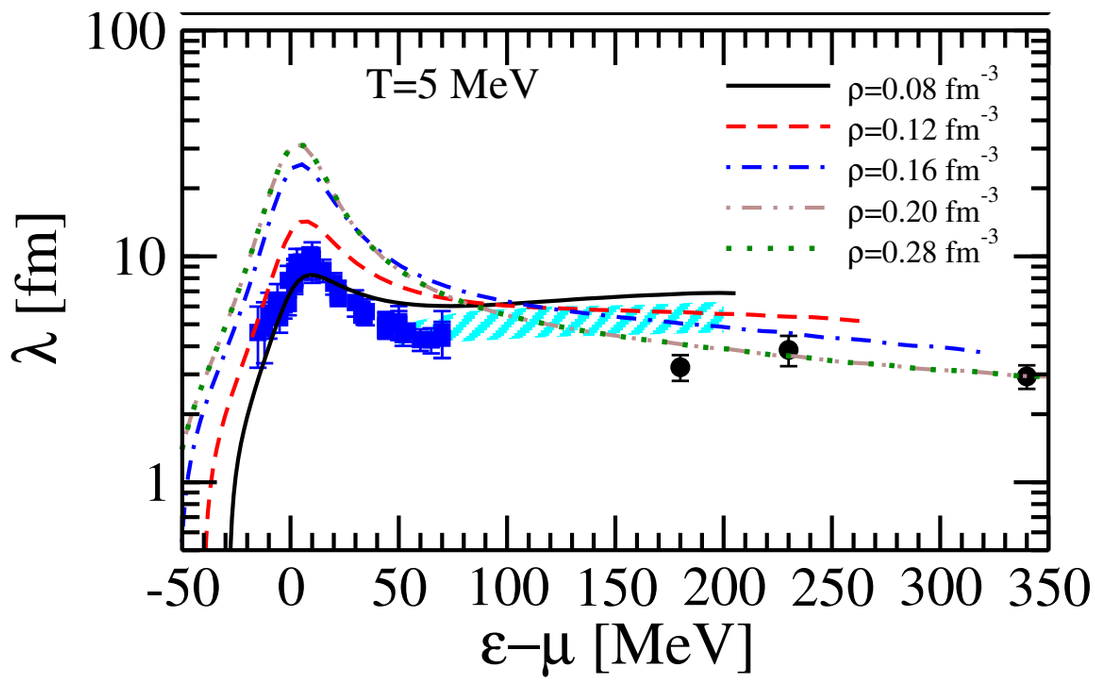
⇓ Turns out that it does

✓ Fermi statistics helps out

✓ Large mean free path λ

→ **Quantum liquid**

[Rios & Somà 2012; Lopez *et al.* 2014]



Liquid drop model & semi-empirical mass formula

⊙ Picture the nucleus as a (suspended) drop of (incompressible) liquid with surface tension

Liquid drop model *[Gamow, Bohr, Weeler]*

Competing processes give rise to nuclear binding

$$\mathrm{BE}(Z,N) = a_v A - a_s A^{2/3} - a_c \frac{Z^2}{A^{1/3}} - a_a \frac{(N-Z)^2}{4A} - \frac{\delta}{A^{1/2}}$$

$A = Z + N$

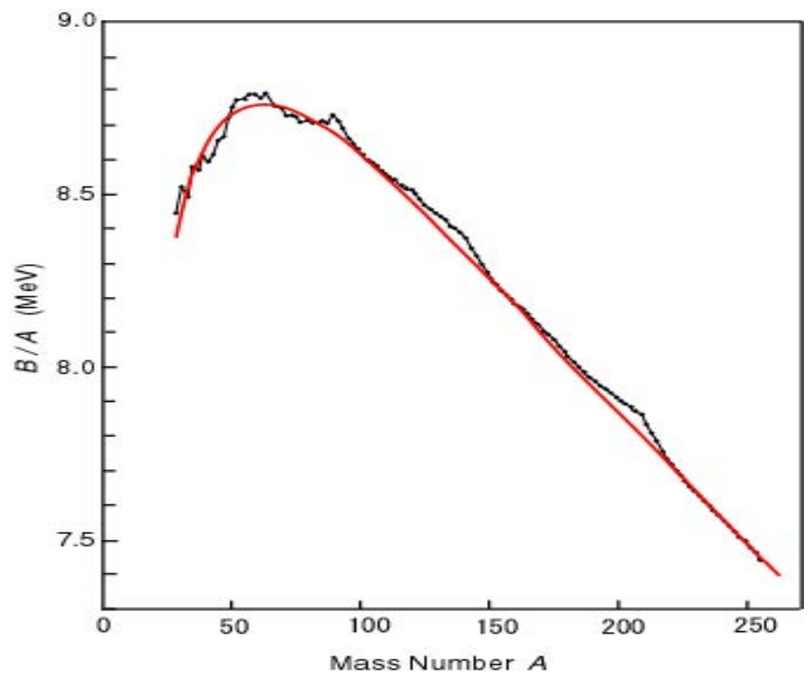
volume — surface — Coulomb — N-Z asymmetry — pairing

1935

[Weizsäcker, Bethe]

✓ Successful in explaining binding energy global trend

✗ Unsuccessful in explaining fine features, excitation spectra, …

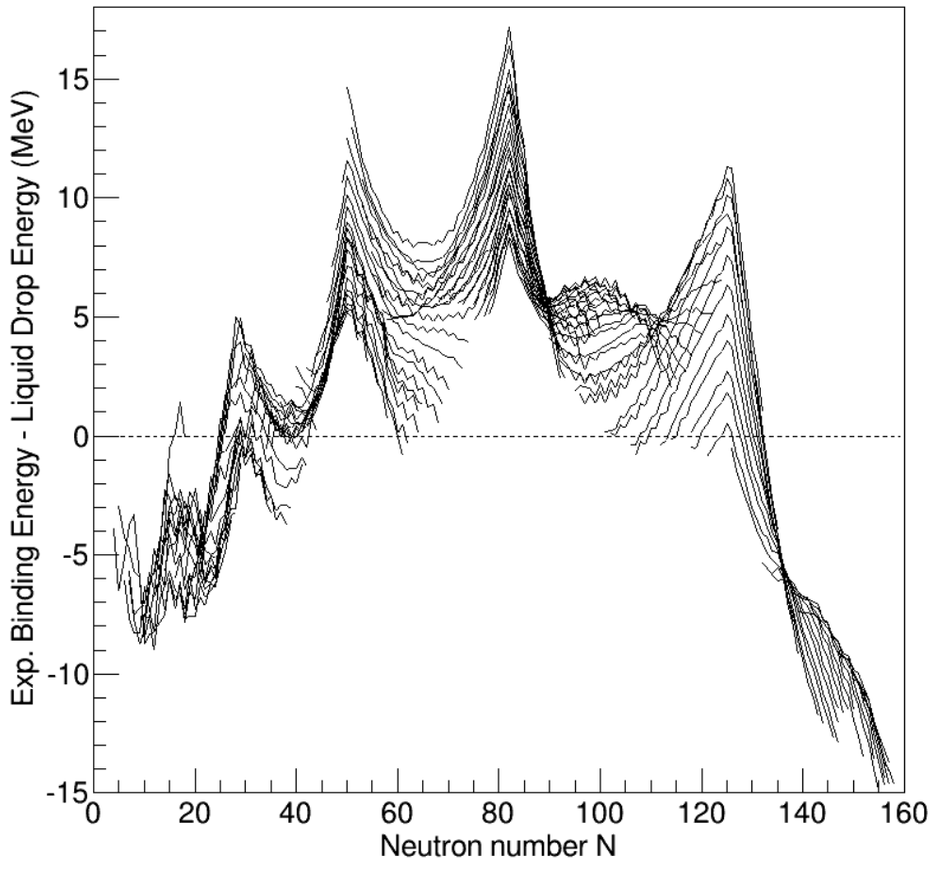


Non-interacting shell model

Measured binding energies
vs.
Liquid drop model predictions

⬇

Systematic deviations



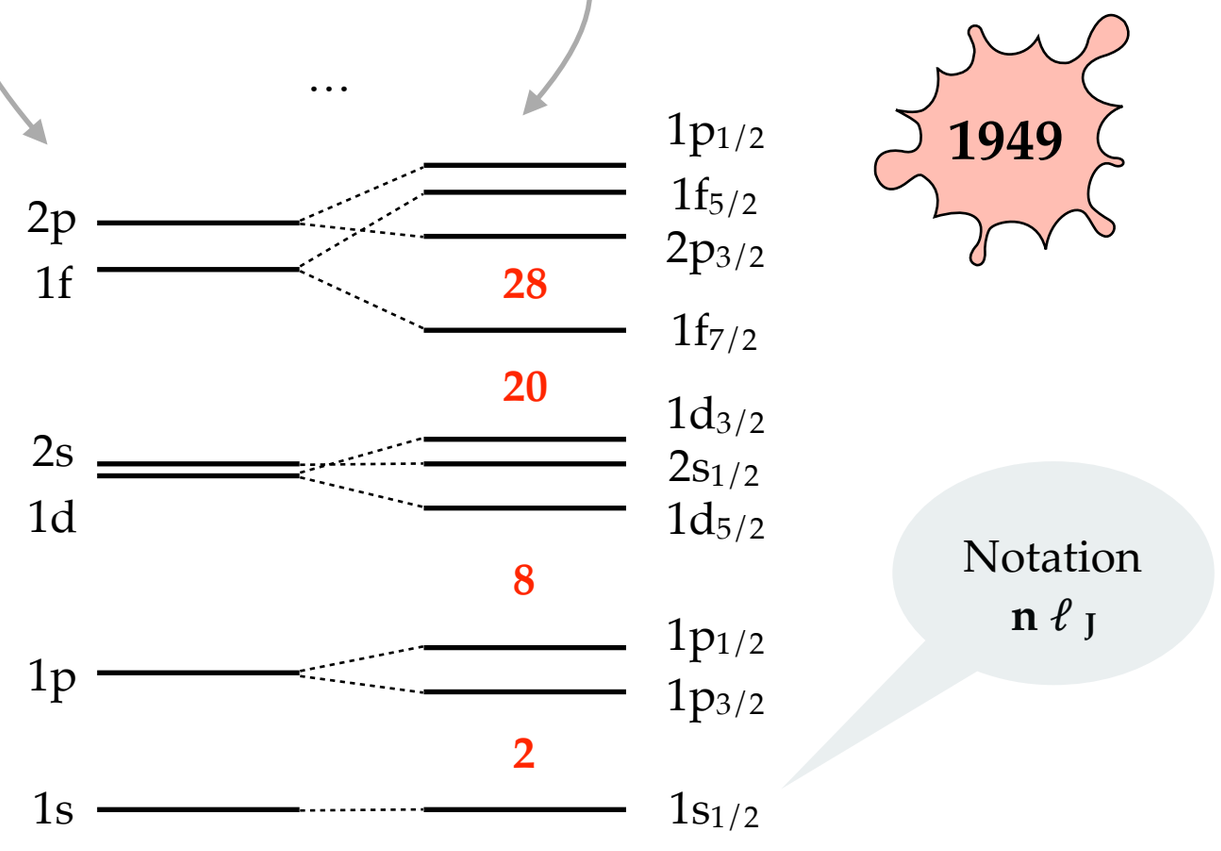
⊙ **What creates regular patterns?**

- Nucleon shells? (cf. electrons in the atom)
- Yet, no obvious common potential

➪ **Idea: devise an effective one-body potential**

- 1. Start with 3D spherical HO potential
- 2. Add term proportional to ℓ^2 (centrifugal)
- 3. Add a spin-orbit term $\ell \cdot s$

[Göppert-Mayer, Jensen]



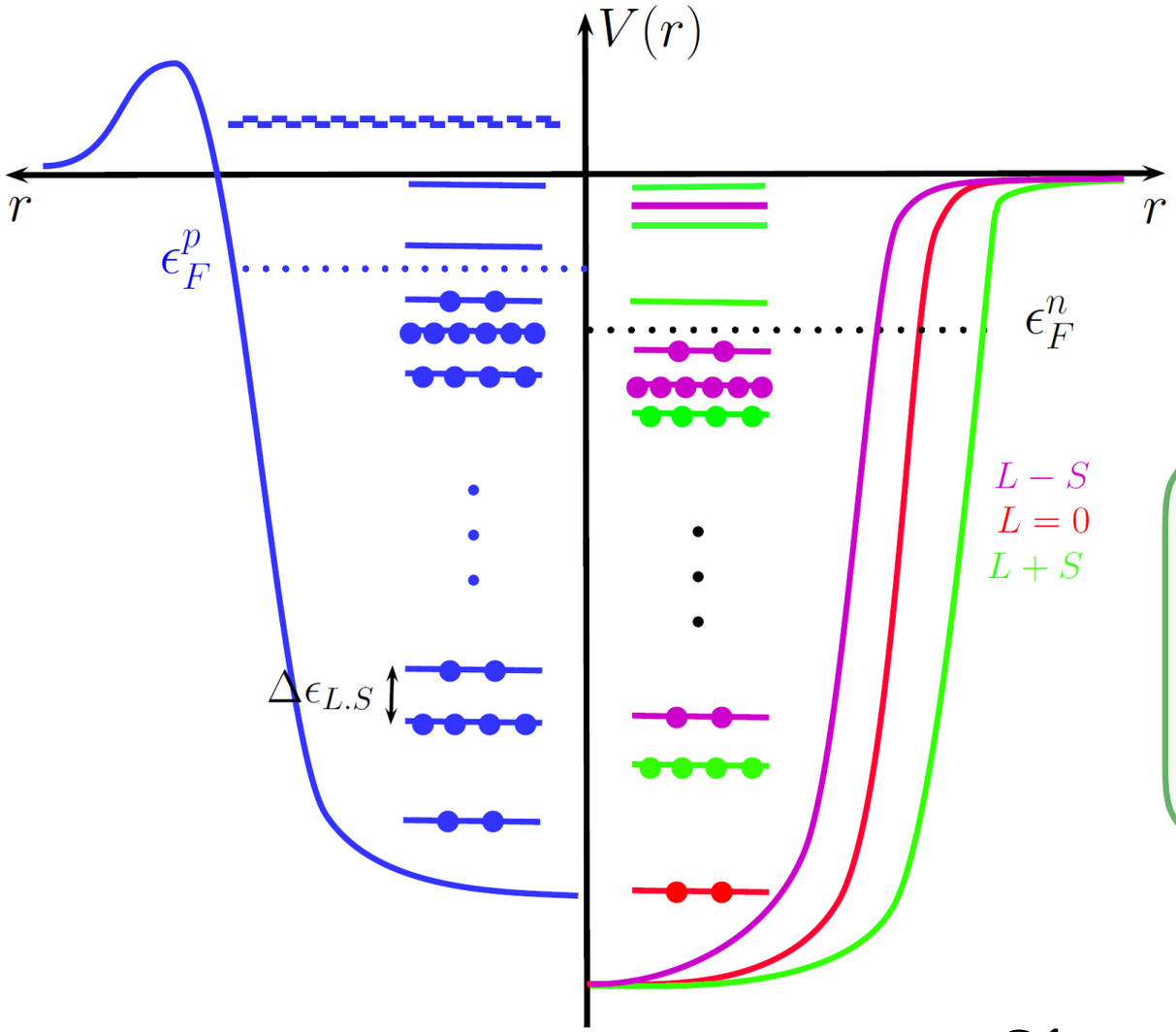
⬇

Magic numbers reproduced!

Empirical mean-field potentials

⊙ **Empirical one-body potentials** provide a reasonable description at a reduced numerical cost

◦ Consider $h(i) = \dfrac{\vec{p}^{\,2}(i)}{2m} + v(i)$ with $v(i) = v(r_i) \equiv -\dfrac{v_0}{1+\exp(\frac{r_i - R}{a})}$



Common parameterisation:
Woods-Saxon (central) potentials

✓ Nucleons placed in single-particle energy levels

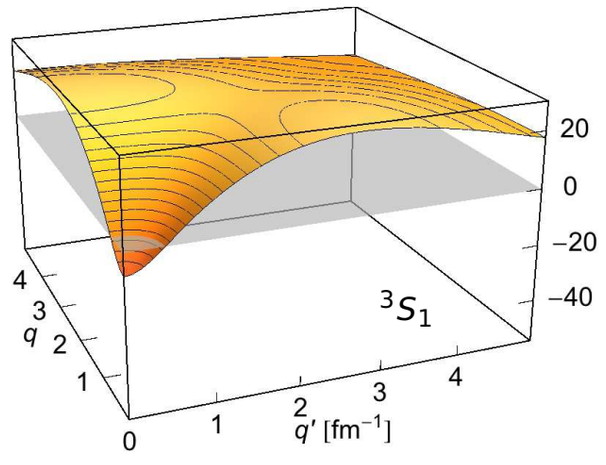
✓ Nucleons fulfil Pauli exclusion principle

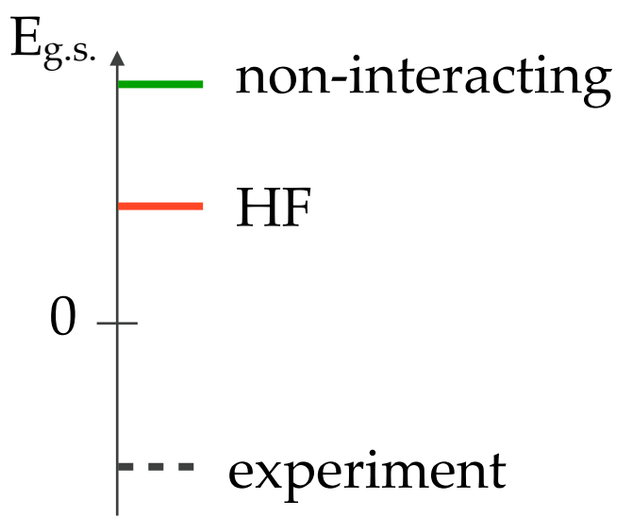
✓ Coulomb shifts proton potentials

➪ Often used in applications needing nuclear physics inputs

Hartree-Fock with realistic potentials

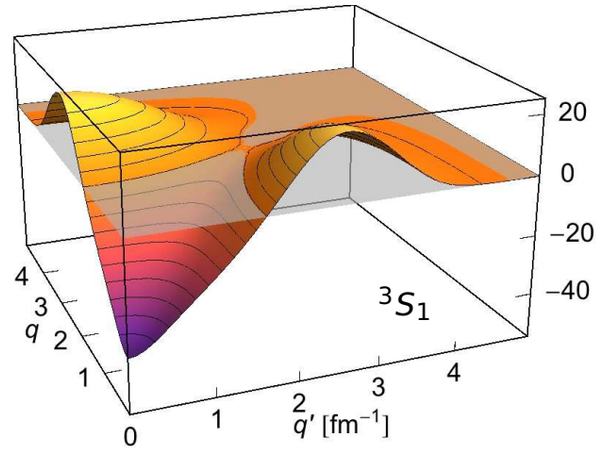
OBE potentials

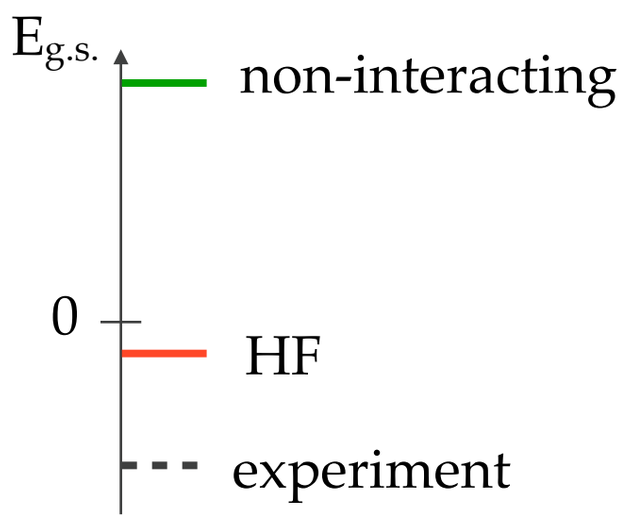




use of expansion method problematic

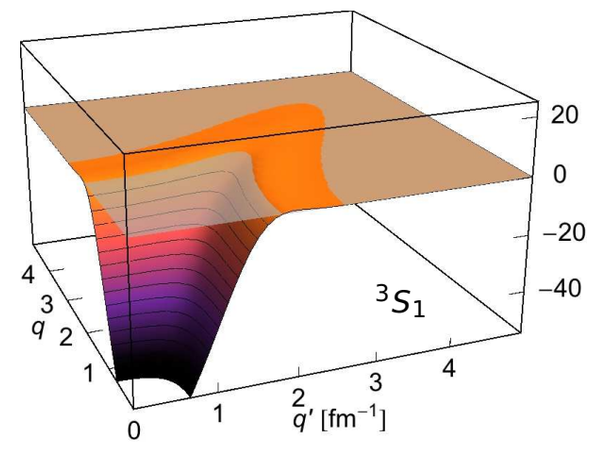
Chiral potentials

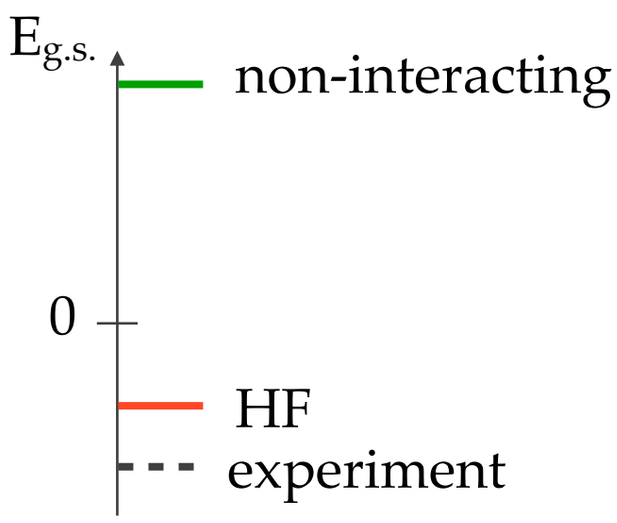




expansion method OK, but problem non-perturbative

SRG potentials





even perturbation theory works!

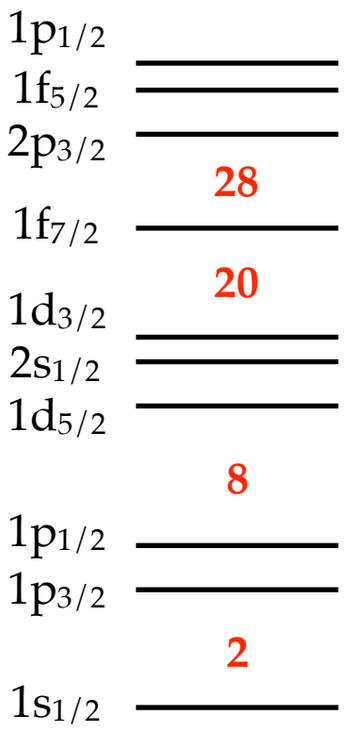
Dynamical vs. static correlations

- **Dynamical**/short-range/weak/single-particle correlations
  - **Dynamical**: characterised by short time scales & high excitation energies
  - **Short-range**: governed by short-distance dynamics
  - **Weak**: perturbative (at least with low-resolution interactions)
  - **Single-particle**: can be described in terms of excitations of a few nucleons
    - ➪ Short-range correlations
    - ➪ Associated with short-range repulsion of NN interactions

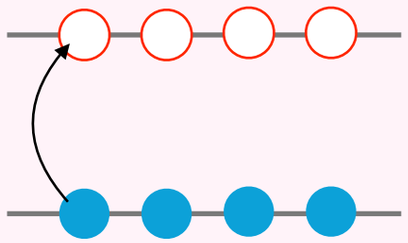
- **Static**/long-range/strong/collective correlations
  - **Static**: characterised by long time scales & low excitation energies
  - **Long-range**: governed by long-distance dynamics
  - **Strong**: strongly non-perturbative
  - **Collective**: description involves coherent excitations of many particles
    - ➪ E.g. pairing or quadrupole correlations
    - ➪ Associated with presence of bound *np* and virtual *nn* pairs (at least pairing correlations)

Closed- vs. open-shell systems

⊙ Mean-field configurations have different features as N and Z vary



Nucleons **entirely** fill levels below a magic number

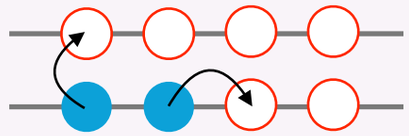


Closed-shell systems

Larger energy gap, excitations hindered, enhanced stability

Dynamical correlations drive bulk properties*

Nucleons **partially** fill levels below a magic number



Open-shell systems

Smaller ($\rightarrow 0$) energy gap, excitations enabled, lesser stability

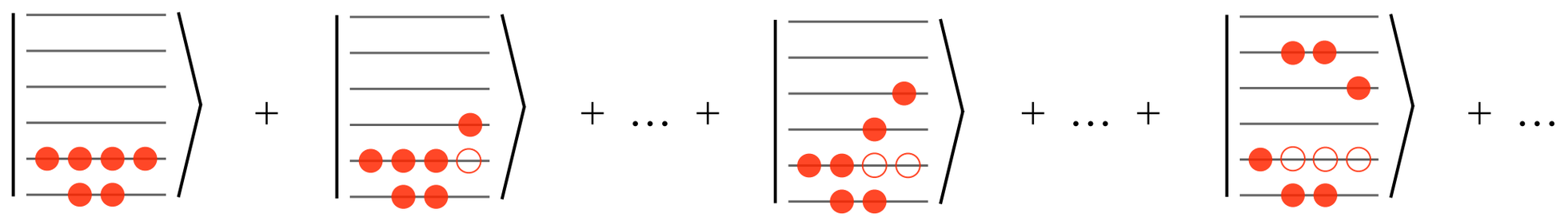
Both static & dynamical correlations are important

*Each observables is impacted differently

Correlations via particle-hole excitations

⊙ In configuration-space methods, correlations are accounted for by means of **ph excitations**

○ Recall: Ref. Slater $|\Phi\rangle \equiv \prod_{i=1}^{A} c_i^\dagger |0\rangle$ → expand on $|\Phi_{ij\ldots}^{ab\cdots}\rangle \equiv c_a^\dagger c_b^\dagger \ldots c_j c_i |\Phi\rangle$



Ref 1p1h 2p2h 3p3h

⊙ **Configuration-interaction techniques** (e.g. no-core shell model)

○ Few-p-few-h and many-p-many-h excitations treated on an equal footing

○ Efficient treatment of both dynamical and static correlations

⊙ **Expansion techniques**

○ Expansion in the rank k of kp-kh excitations

○ Efficient treatment of **dynamical** correlations, difficult to treat **static** correlations

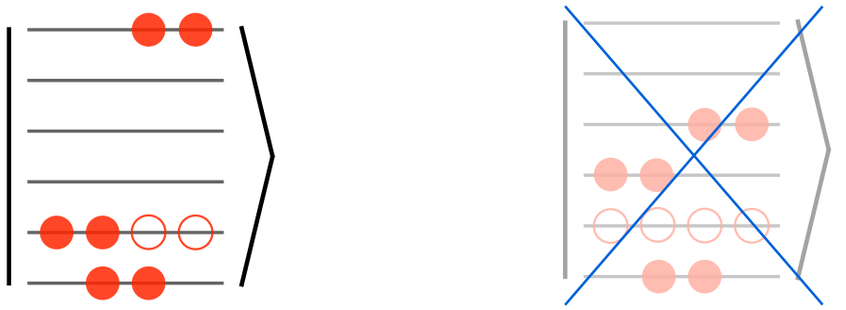
Correlations via particle-hole excitations

- The two different strategies reflect into two different truncations of the Hilbert space
- **Configuration-interaction techniques**
  - Truncation in terms of the total number of HO excitation quanta $N_{\max}$ of the many-body states

E.g. $N_{\max} = 6$ calculation
No-core shell model

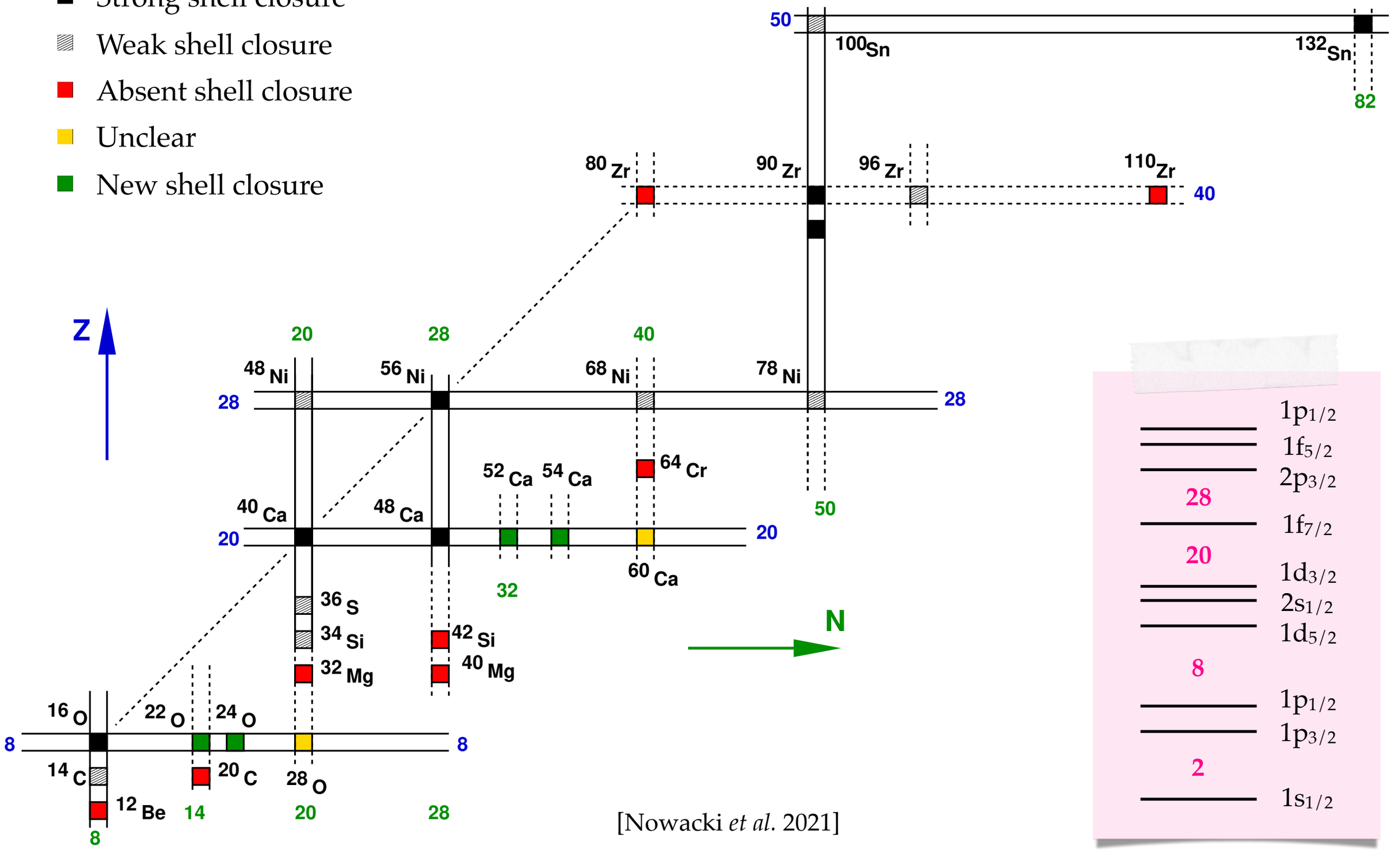
- **Expansion techniques**
  - Truncation in terms of the energy of the states included in the one-body basis
  - (On top of this there's the truncation on the rank k of kp-kh excitations that are included)

E.g. $e_{\max} = 6$ calculation
2p2h truncation



Closed vs. open shells

- Strong shell closure
- Weak shell closure
- Absent shell closure
- Unclear
- New shell closure



[Nowacki *et al.* 2021]

Contents

Formal perturbation theory

- Very popular in description of **many-electron systems** (since early days)
  - Coulomb interaction sufficiently weak to allow perturbative treatment
- **Applications in many-nucleon systems traditionally hindered by strong short-range repulsion**
  - SRG techniques have completely changed this view → renaissance of MBPT in nuclear physics
- **Starting point: splitting of the many-body Hamiltonian ("partitioning")**

$$H \equiv H_0 + H_1$$

unperturbed — perturbation

  - Eigenvalue equation for H_0 must be **numerically accessible**

$$H_0|\Phi_k\rangle = E_k^{(0)}|\Phi_k\rangle \quad \rightarrow \text{ set of unperturbed eigenstates and eigenenergies} \quad \{|\Phi_k\rangle, E_k^{(0)}; k \in \mathbb{N}\}$$

form orthonormal basis of Hilbert space

  - In the following $|\Psi_0^{\mathrm{A}}\rangle = |\Psi^{\mathrm{A}}\rangle \qquad |\Phi_0\rangle = |\Phi\rangle \qquad E_0^{(0)} = E^{(0)}$
- **Goal: approach exact (g.s.) wave function and energy by systematically including effects of H_1**

Formal perturbation theory

⊙ Define **projectors** associated with the partitioning of H

$$P \equiv |\Phi\rangle\langle\Phi| \qquad Q \equiv 1 - P \qquad \text{with} \qquad P|\Phi\rangle = |\Phi\rangle \qquad Q|\Phi\rangle = 0$$

$$\rightarrow \; Q \text{ can be written as} \qquad Q \equiv \sum_k{}' |\Phi_k\rangle\langle\Phi_k| \equiv \sum_{|\Phi_k\rangle \neq |\Phi\rangle} |\Phi_k\rangle\langle\Phi_k|$$

⊙ **Express the exact wave function as**

$$|\Psi^{\mathrm{A}}\rangle = P|\Psi^{\mathrm{A}}\rangle + Q|\Psi^{\mathrm{A}}\rangle$$
$$= |\Phi\rangle + |\chi\rangle$$

unperturbed wave function — correlated wave function

⊙ It follows that the exact energy can be written as

$$E^{\mathrm{A}} = \langle\Phi|H|\Psi^{\mathrm{A}}\rangle$$
$$= \underbrace{\langle\Phi|H_0|\Phi\rangle + \langle\Phi|H_1|\Phi\rangle}_{\equiv E_{\mathrm{ref}}} + \underbrace{\langle\Phi|H_1|\chi\rangle}_{\equiv \Delta E}$$

reference energy — **correlation energy**

Formal perturbation theory

- Introduce **resolvent operator**

$$R^{\mathrm{RS}} \equiv \sum_k{}' \frac{|\Phi_k\rangle\langle\Phi_k|}{E^{(0)} - E_k^{(0)}}$$

Rayleigh-Schrödinger

which has the property $R^{\mathrm{RS}}|\Phi\rangle = 0$

- Finally, one gets

$$|\chi\rangle = \sum_{k=1}^{\infty} (RH_1)^k |\Phi\rangle_c \qquad \textbf{correlated wave function}$$

$$\Delta E = \langle\Phi|H_1 \sum_{k=1}^{\infty} (RH_1)^k |\Phi\rangle_c \qquad \textbf{correlation energy}$$

and can write exact wave function and g.s. energy as **power series in H_1**

$$|\Psi^{\mathrm{A}}\rangle \equiv \sum_{p=0}^{\infty} |\Psi^{(p)}\rangle \qquad E^{\mathrm{A}} \equiv \sum_{p=0}^{\infty} E^{(p)}$$

e.g.

$$E^{(2)} = \sum_k{}' \frac{\langle\Phi|H_1|\Phi_k\rangle\langle\Phi_k|H_1|\Phi\rangle}{E^{(0)} - E_k^{(0)}}$$

Many-body perturbation theory

- **Application to many-nucleon systems**
  - Characterise unperturbed Hamiltonian
  - Define basis, derive working expressions (many-body matrix elements & unperturbed energies)
  - Use Wick's theorem → many-body diagrams

- **Reference state: Slater determinant**

$$|\Phi\rangle \equiv \prod_{i=1}^{A} c_i^\dagger |0\rangle$$

- **Normal-ordered Hamiltonian**

NO2B approximation

  - Apply Wick's theorem with respect to the reference Slater to H

$$H = H^{[0]} + \sum_{pq} H^{[2]}_{pq} \, :c_p^\dagger c_q: + \frac{1}{4} \sum_{pqrs} H^{[4]}_{pqrs} \, :c_p^\dagger c_q^\dagger c_s c_r: + \ldots$$

  - Effective (normal-ordered) operators
  - Each NO operator of rank $\boldsymbol{k_{\mathrm{eff}}}$ receives contributions from original operators with $\boldsymbol{k_{\mathrm{eff}} \leq k \leq k_{\mathrm{max}}}$

Many-body perturbation theory

⊙ **Partitioning**

○ Add and subtract a diagonal (NO) one-body operator

$$H_0 = H^{[0]} + \sum_p e_p \, :c_p^\dagger c_p:$$

$$H_1 \equiv \breve{H}^{[2]} + H^{[4]}$$

with

$$\bar{H}^{[2]} \equiv \sum_p e_p \, :c_p^\dagger c_p$$

$$\breve{H}^{[2]} \equiv H^{[2]} - \bar{H}^{[2]} = \sum_{p \neq q} H_{pq}^{[2]} \, :c_p^\dagger c_q:$$

⊙ Recall: an **orthonormal basis of the *A*-body Hilbert space** can be built via Slater determinants

$$\mathcal{H}^A = \{|\Phi\rangle, |\Phi_i^a\rangle, |\Phi_{ij}^{ab}\rangle, |\Phi_{ijk}^{abc}\rangle, ...\} \qquad \text{where} \quad |\Phi_{ij\ldots}^{ab\cdots}\rangle \equiv c_a^\dagger c_b^\dagger \ldots c_j c_i |\Phi\rangle$$

→ eigenbasis of H_0

$$H_0|\Phi\rangle = H^{[0]}|\Phi\rangle$$

$$H_0|\Phi_{ij\ldots}^{ab\cdots}\rangle = (H^{[0]} + \epsilon_{ij\ldots}^{ab\cdots})|\Phi_{ij\ldots}^{ab\cdots}\rangle$$

with $\epsilon_{ij\ldots}^{ab\cdots} \equiv (e_a + e_b + \cdots) - (e_i + e_j + \cdots)$

○ **Convention**: one-body states occupied (unoccupied) in the reference determinant are labeled by i,j,k, … (a,b,c, …) and are referred to as **hole** (**particle**) states

Many-body perturbation theory

⊙ **Choice of partitioning**

○ Simplest choice in nuclear physics: HO Hamiltonian $H_0 \equiv \frac{\vec{p}^{\,2}}{2m} + \frac{1}{2} m\omega^2 \vec{r}^{\,2}$

○ Common (more refined) choice: **Hartree-Fock reference**

→ Solve variational HF problem and build $\bar{H}^{[2]}$ from one-body HF Hamiltonian

→ **Møller-Plesset partitioning** $\breve{H}^{[2]} = 0 \rightarrow H_1 = H^{[4]}$

⊙ **Resolvent operator**

$$R = -\sum_{ai} \frac{|\Phi_i^a\rangle\langle\Phi_i^a|}{\epsilon_i^a} - \left(\frac{1}{2!}\right)^2 \sum_{abij} \frac{|\Phi_{ij}^{ab}\rangle\langle\Phi_{ij}^{ab}|}{\epsilon_{ij}^{ab}} - \left(\frac{1}{3!}\right)^2 \sum_{abcijk} \frac{|\Phi_{ijk}^{abc}\rangle\langle\Phi_{ijk}^{abc}|}{\epsilon_{ijk}^{abc}} + \ldots$$

⊙ **Second-order energy correction**

$$E^{(2)} = -\sum_{ai} \frac{H_{ai}^{[2]} H_{ia}^{[2]}}{\epsilon_i^a} - \frac{1}{4} \sum_{abij} \frac{H_{abij}^{[4]} H_{ijab}^{[4]}}{\epsilon_{ij}^{ab}}$$

Computational advantages

○ No computation of Hamiltonian matrix

○ Non-iterative calculation

○ Polynomial scaling $O(N^4)$

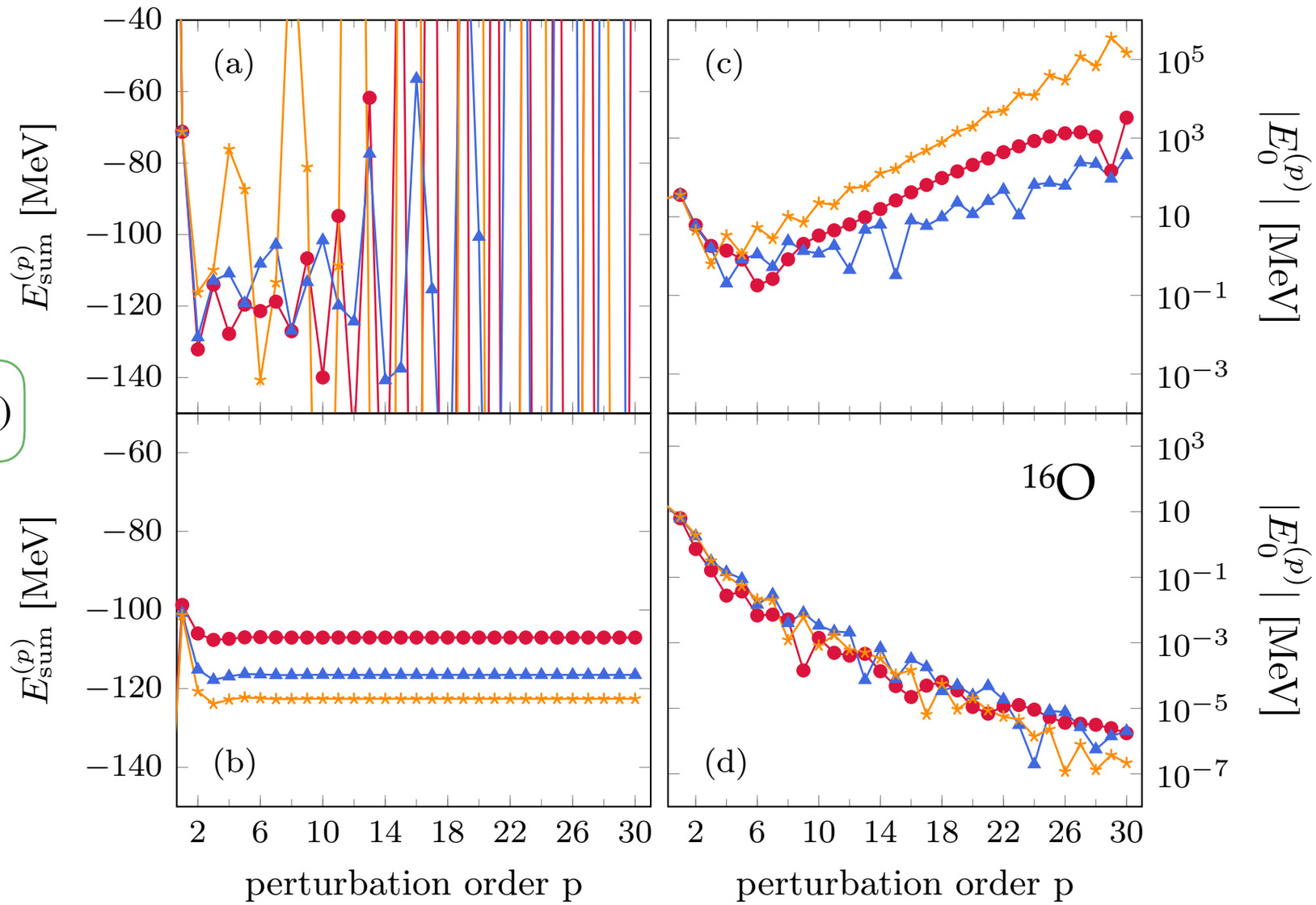
Many-body perturbation theory

- **Convergence of MBPT series**
  - Convergence of the series can be tested up to high orders in small basis (recursive scheme)
  - Importance of using the right reference
  - Resummation schemes possible (e.g. Padé, eigenvector continuation, …)

HO reference

$N_{\max}$ = 2 (●), 4 (▲) and 6 (★)

HF reference



[Tichai *et al.* 2016]

Many-body perturbation theory

⊙ **Choice of SRG parameter**

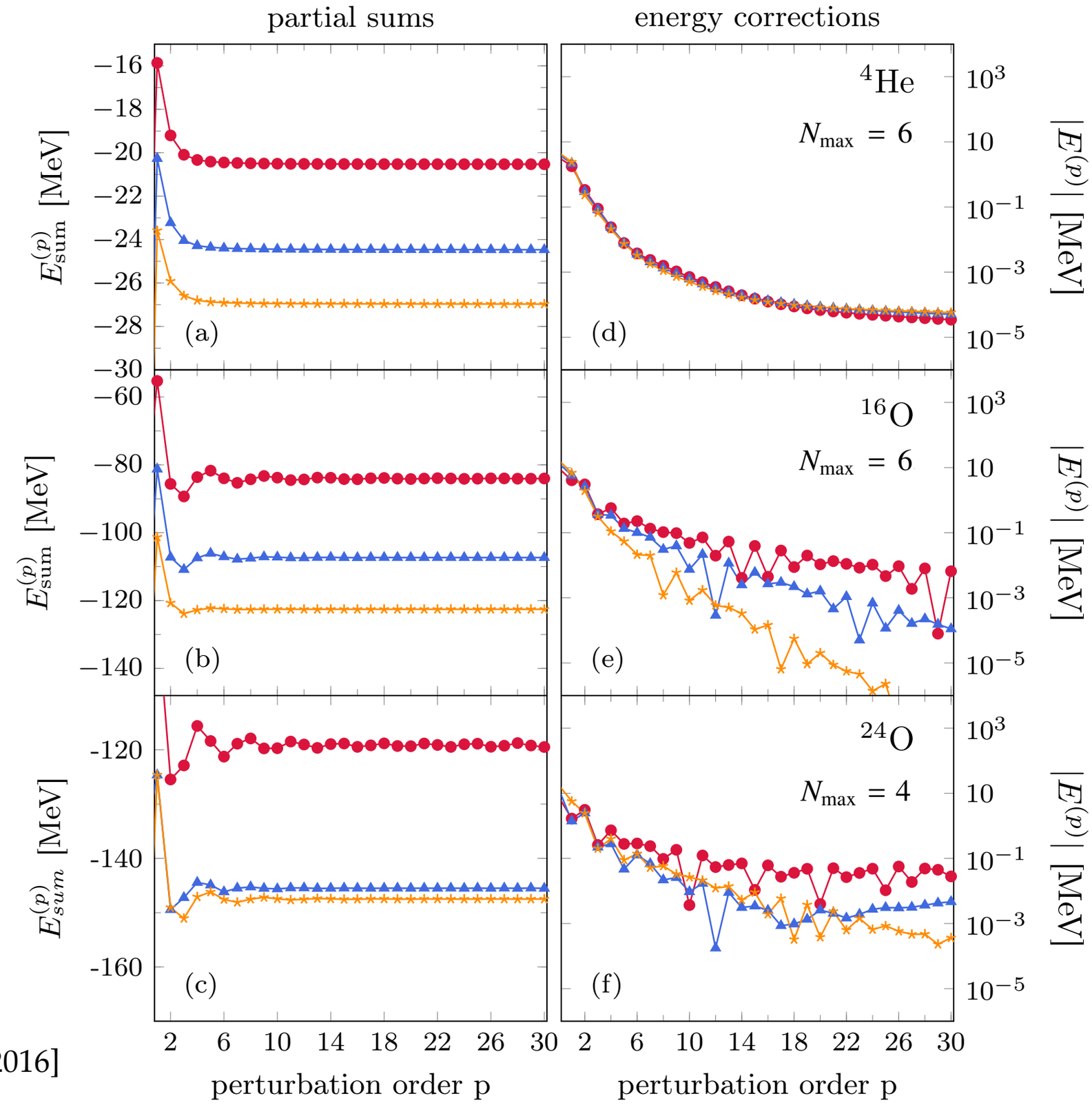
○ Convergence rate depends on α

$\alpha = 0.02\,\mathrm{fm}^4$ (●)

$0.04\,\mathrm{fm}^4$ (▲)

$0.08\,\mathrm{fm}^4$ (★)

○ Additional $N_{\max}$ dependence



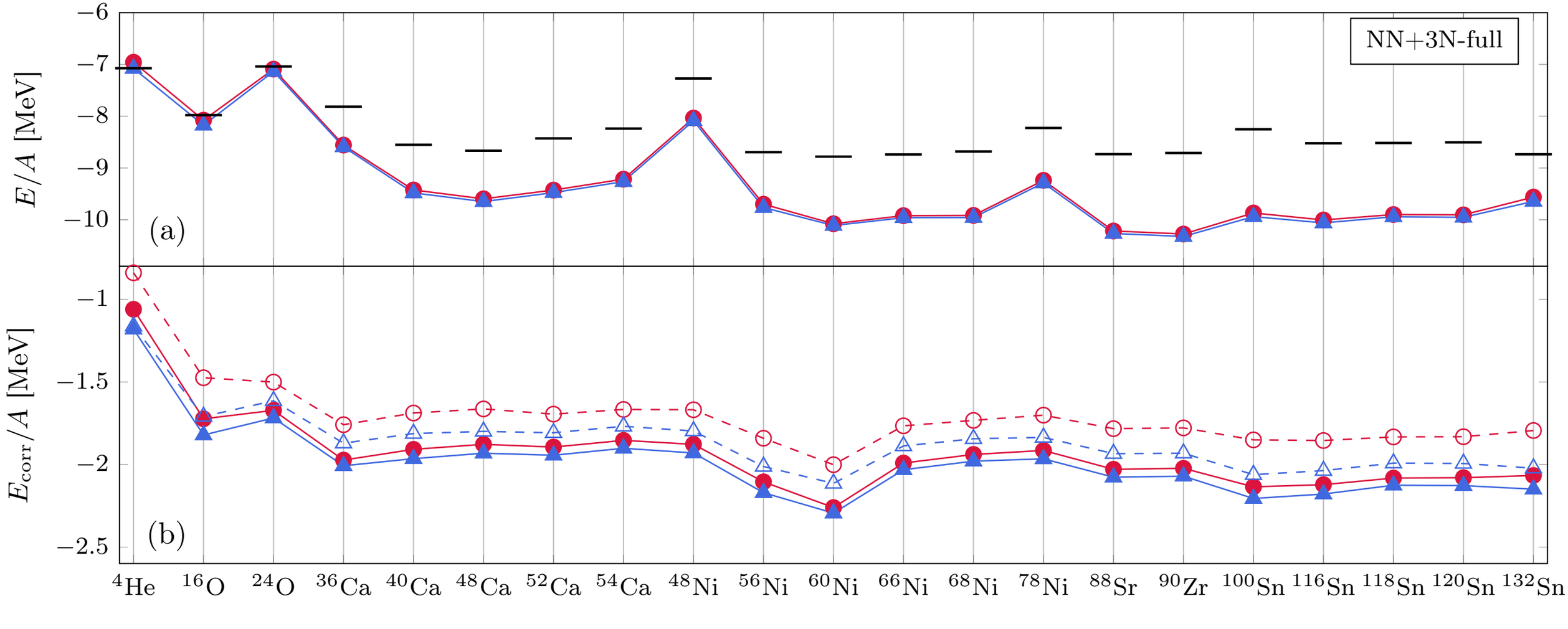
[Tichai *et al.* 2016]

Many-body perturbation theory

- **Reach**
  - Calculations currently possible up to mass $A \sim 100$ (and beyond)
- **Benchmark** [Tichai *et al.* 2016]
  - Accuracy competitive to coupled cluster calculations (non-perturbative and more costly)

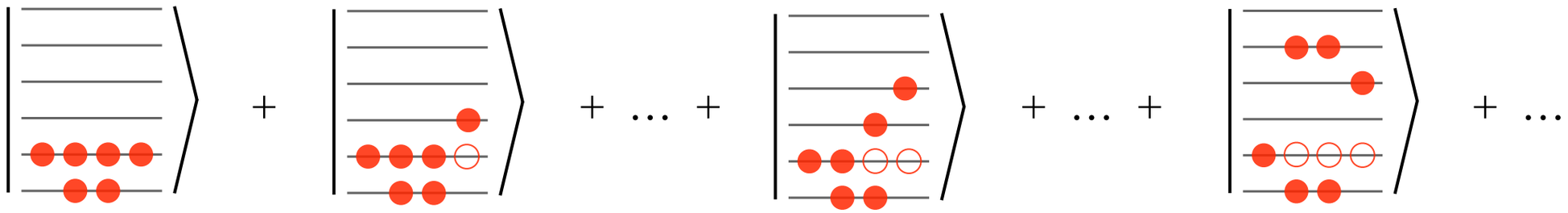
MBPT $E_0^{(2)}$ (○) $E_0^{(2)} + E_0^{(3)}$ (●)

Coupled cluster CCSD (△) CR-CC(2,3) (▲)



Non-perturbative methods

⊙ **Expansion of the exact wave function**

$$|\Psi_0^A\rangle =$$  $$+ \ \ldots \ +$$ $$+ \ \ldots \ +$$ $$+ \ \ldots$$

Ref 1p1h 2p2h 3p3h

➪ **Perturbative** methods: expansion coefficients computed **independently**

➪ **Non-perturbative** methods: expansion coefficients computed **self-consistently**

➪ **Truncated CI**: expansion coefficients computed **via a diagonalisation**

⊙ Examples of non-perturbative approaches

○ **Coupled-cluster theory (CC)**

➪ Exponential ansatz for the wave function $|\Psi_{CC}\rangle = e^T |\Phi\rangle$

○ **In-medium similarity renormalisation group (IMSRG)**

➪ SRG evolution for H normal-ordered w.r.t. to a reference Slater determinant

Green's function techniques

⊙ The goal is to solve the ***A*-body Schrödinger equation**

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

⊙ Instead of working with the full A-body wave function $|\Psi_k^A\rangle$, rewrite the Schrödinger equation in terms of **1-, 2-, …. *A*-body objects** G_1=G, G_2, … G_A (**Green's functions**)

➟ A-1 coupled equations

⊙ 1-, 2-, …. A-body Green's functions yield **expectation values of 1-, 2-, …. *A*-body operators**

➟ In practice, one usually needs 1- and/or 2-body GFs (~ 1- & 2-body density matrices)

⊙ One-body Green's function obtained by solving **Dyson equation** (derived from Schrödinger eq.)

$$G = G^{(0)} + G^{(0)}\,\Sigma\,G$$

unperturbed Green's function

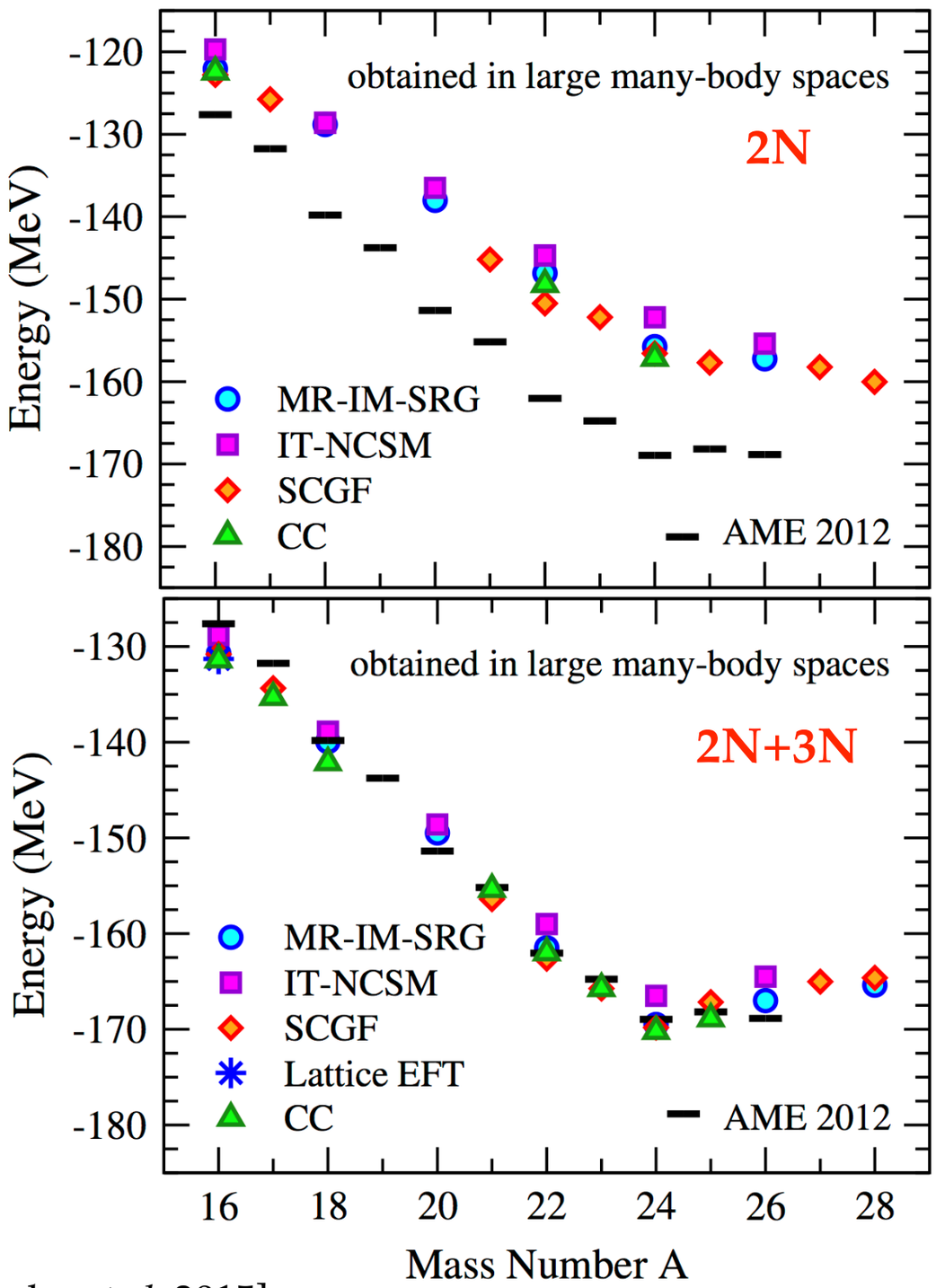
many-body effects contained in the **self-energy** Σ

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

➟ Spectral or **Lehmann representation** of the Green's function

Benchmarks

Oxygen binding energies



[Hebeler *et al.* 2015]

⊙ **Convergence of many-body results**

- ○ Different strategies to solve $H\Psi=E\Psi$
- ○ Same input Hamiltonian (except lattice EFT)
- ○ **All methods agree within 5%**

⊙ **Physics of oxygen isotopes**

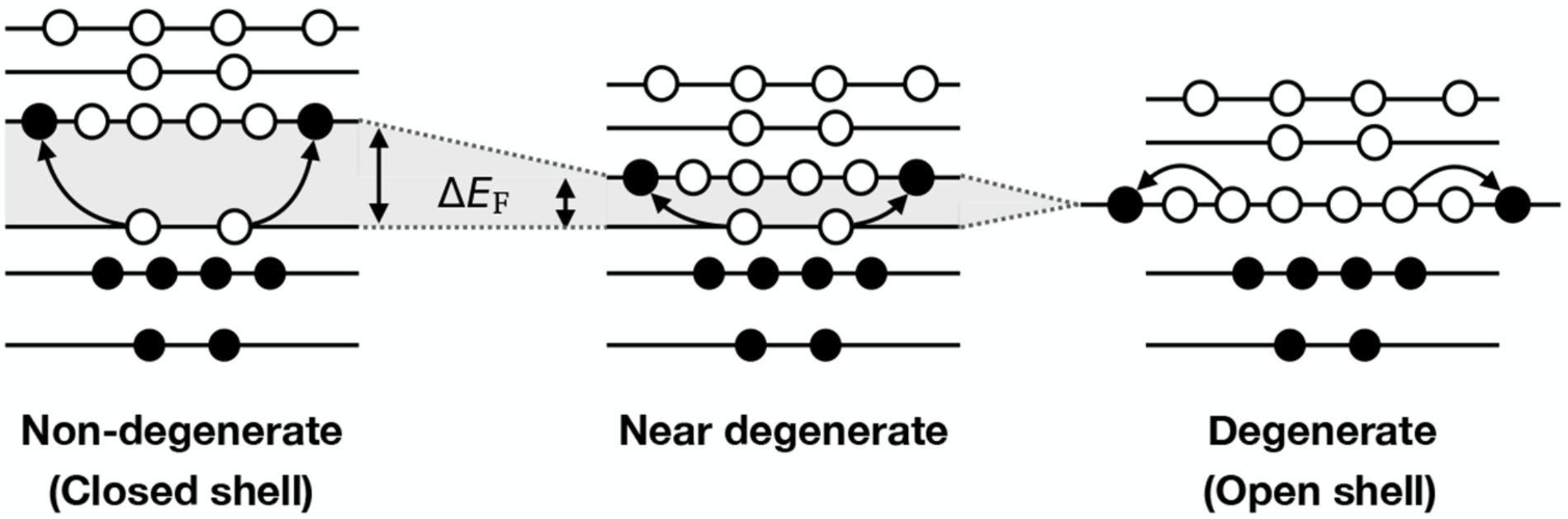
- ○ Energy trend reproduced by 2N+3N results
- ○ **Correct drip line only with 3N forces**

Contents

Degeneracy of open-shell systems

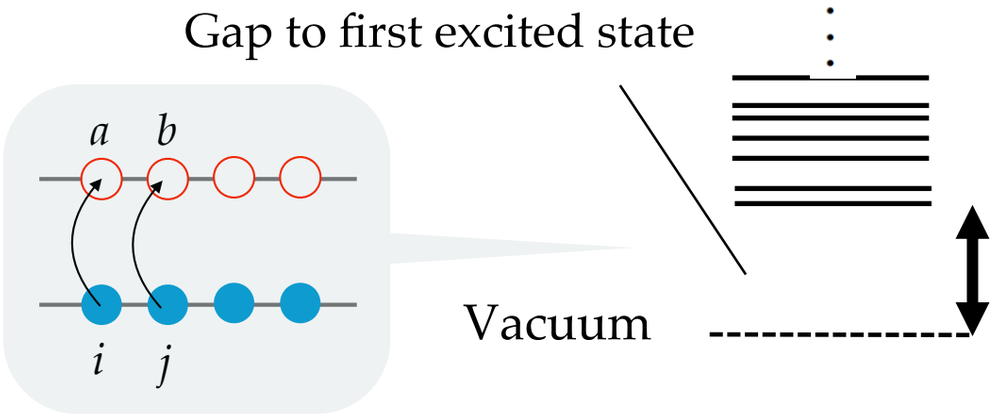
- **Configuration-space methods expand the solution in ph excitations on top of a reference state**
  - Standard formulation: reference state has the same symmetries of the exact wave function
  - Very efficient to account for dynamical (weak) correlations → closed-shell nuclei
  - What about static (strong) correlations? → open-shell nuclei

- Open-shell nuclei are **(near-)degenerate** with respect to ph excitations
  - Gap at the Fermi surface decreases (→ 0 in the limit)
  - ph hierarchy becomes ill-defined



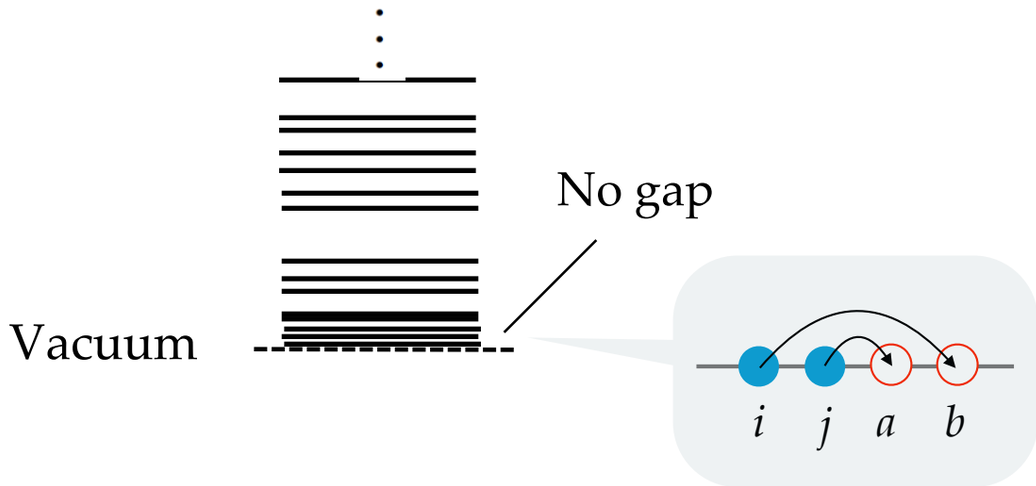
Breakdown of ph expansion

Closed-shell



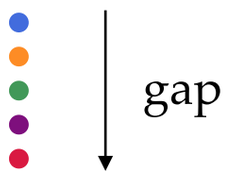
$$\Delta E^{(2)}_{\mathrm{MBPT}} = -\frac{1}{4}\sum_{ijab}\frac{|h^{(2)}_{ijab}|^2}{e_a + e_b - e_i - e_j} > 0$$

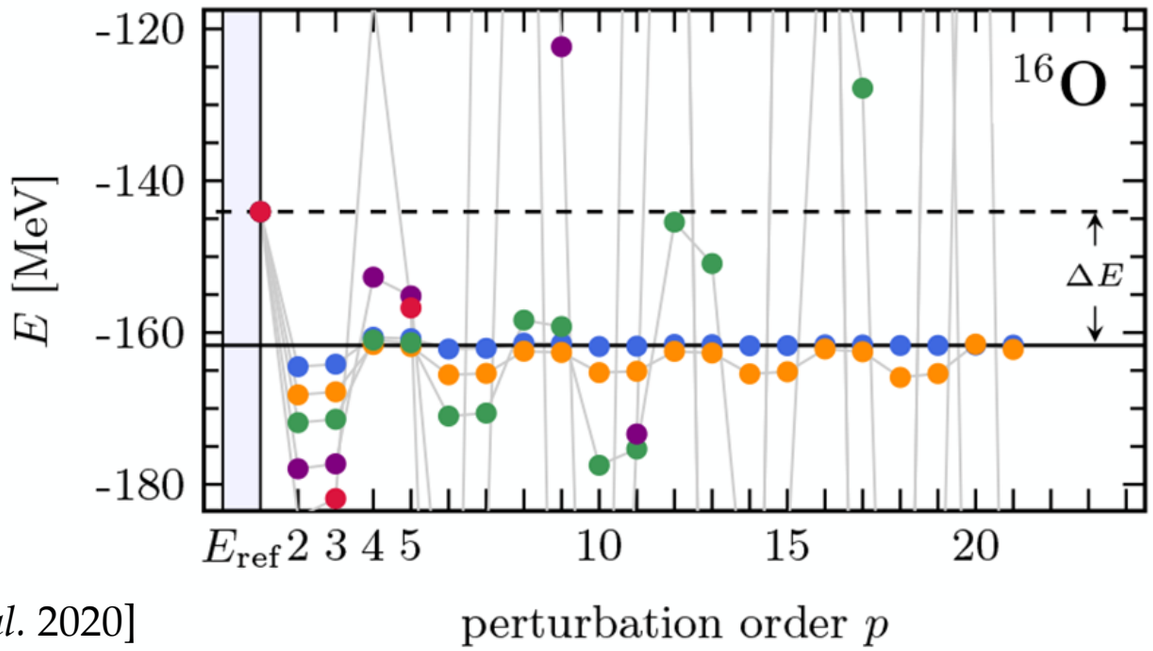
Open-shell



$$\Delta E^{(2)}_{\mathrm{MBPT}} = -\frac{1}{4}\sum_{ijab}\frac{|h^{(2)}_{ijab}|^2}{e_a + e_b - e_i - e_j} = 0$$

- Breakdown of ph expansion evident already in MBPT(2) expressions
- Can be explicitly demonstrated by artificially decreasing the gap in ^{16}O



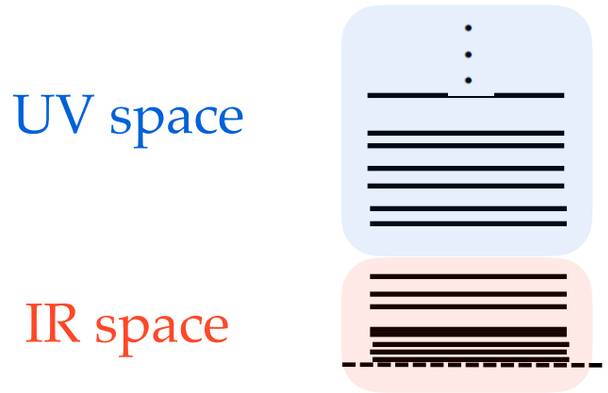


[Tichai *et al.* 2020]

Single- vs multi-reference strategy

⊙ **Multi-reference** strategy

- ○ Reopens the gap via **IR diagonalisation**
- ○ Ref: linear combination of Slater dets.
- ○ UV correlations via ph excitations



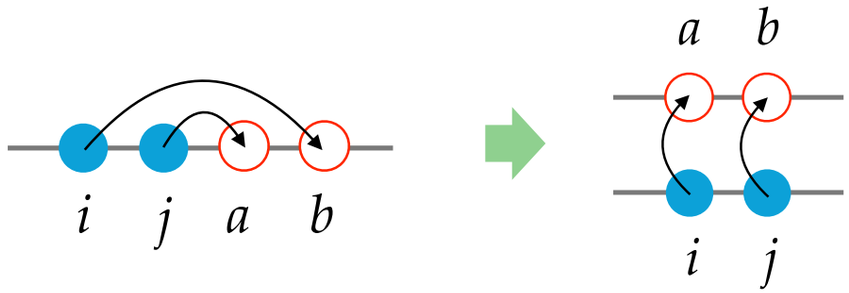
$$|\Psi_0^{J=0\,A}\rangle = \Omega_0^{UV}|\Theta_{0\,IR}^{J=0\,A}\rangle$$

✓ Symmetries are automatically preserved

✗ ph expansion: complicated formalism

⊙ **Single-reference** strategy

- ○ Reopens the gap via **symmetry breaking**
- ○ Ref: single Slater determinant
- ○ UV correlations via ph excitations



$$|\Psi_0^{J=0\,A}\rangle = \Omega_0^{SB}|\Phi_0^{SB}\rangle$$

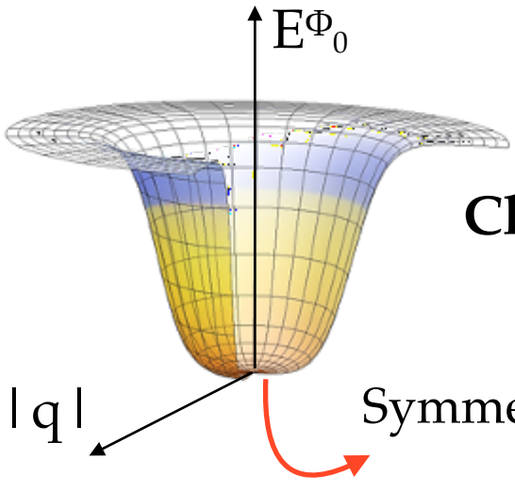
✓ ph expansion: simpler formalism

✗ Symmetries must be restored

Symmetry breaking

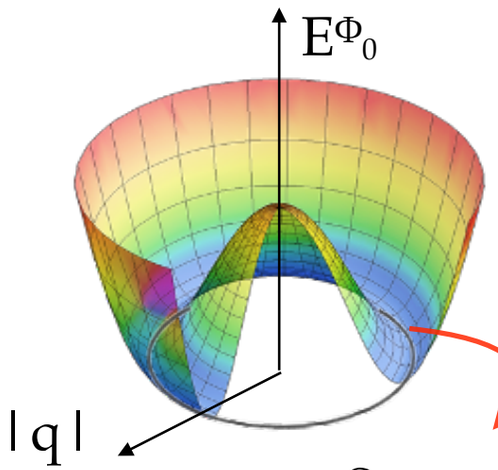
- **Enlarge the variational space**
  - Requiring the w.f. ansatz to have the same symmetries of H is too restrictive
  - In most cases, mean-field solution spontaneously breaks symmetries if allowed

- **Lift the degeneracy**
  - Trade the ph degeneracy for one in the transformations of the associated symmetry group
  - Order parameter $\langle\Phi_0|Q|\Phi_0\rangle = q \equiv |q|e^{i\arg(q)}$



Closed-shell systems

Symmetry-conserving minimum



Open-shell systems

Symmetry-breaking minimum

- **Symmetry restoration**
  - Symmetry breaking is **fictitious** in finite systems
  - Symmetry breaking is an intermediate step → symmetries must be **restored** at the end

Symmetry breaking

⊙ Which symmetries **can** be broken?

Physical symmetry	**Group**	**Casimir**	**Correlations**
Rotational inv.	SU(2)	$\hat{\vec{J}}^2$	Deformation
Particle-number inv.	$U(1)_N$ x $U(1)_Z$	$\hat{N}$, $\hat{Z}$	Pairing

⊙ Which symmetries **should** be broken?

○ In principle, the more the better (provided calculations are feasible)

○ In practice, there are different formal & computational consequences

➪ Breaking U(1) requires a modification of the (bases of the) formalism, breaking SU(2) doesn't

➪ Computationally, breaking U(1) is cheaper than breaking SU(2) (**symmetry reduction**)

U(1)-breaking methods were first developed

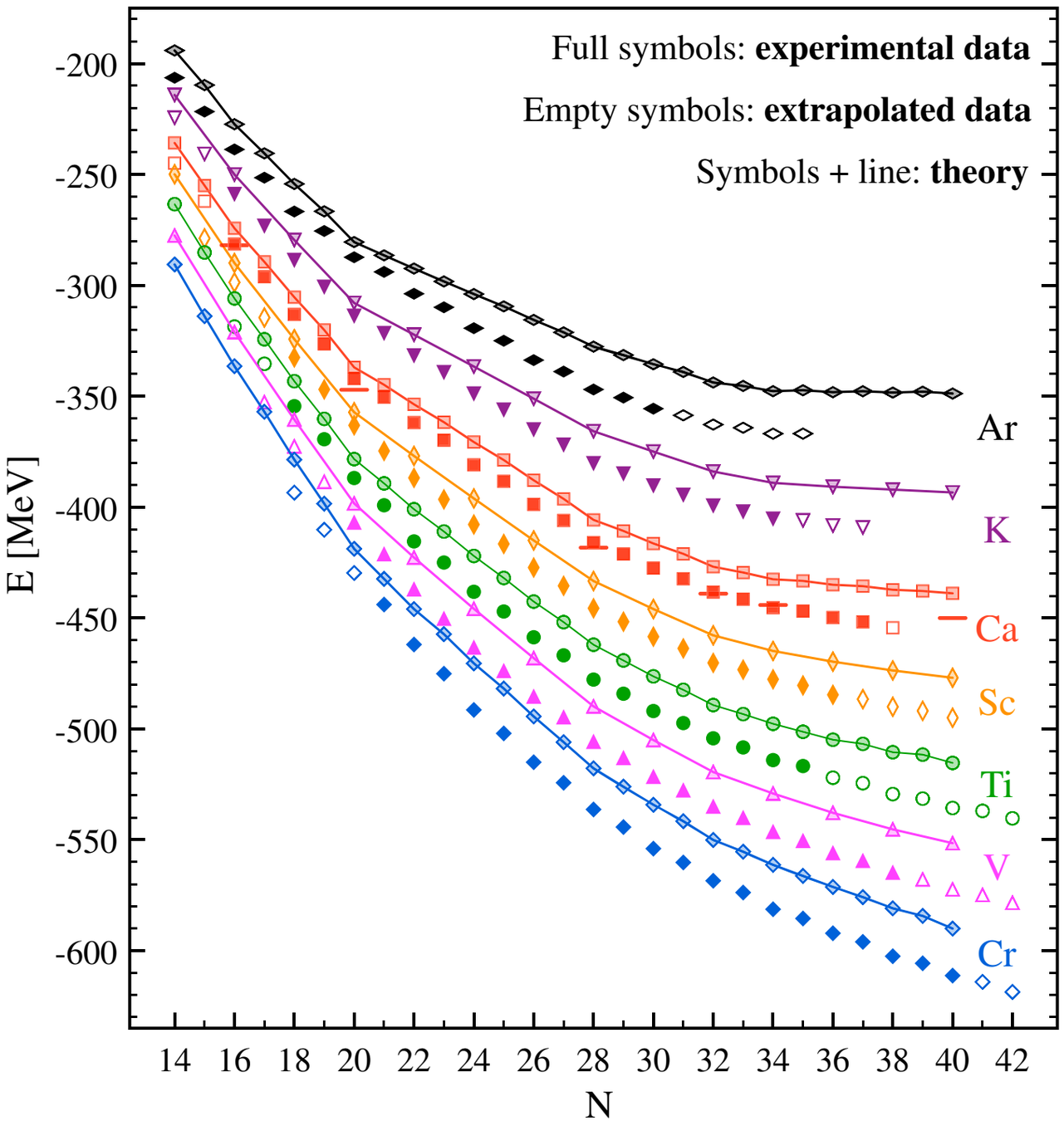
○ Ultimately, it depends on the system

○ **Singly open-shell** nuclei ➪ Sufficient to **break U(1)**

○ **Doubly open-shell** nuclei ➪ Necessary to **break SU(2)**

Contents

Gorkov Green's function theory



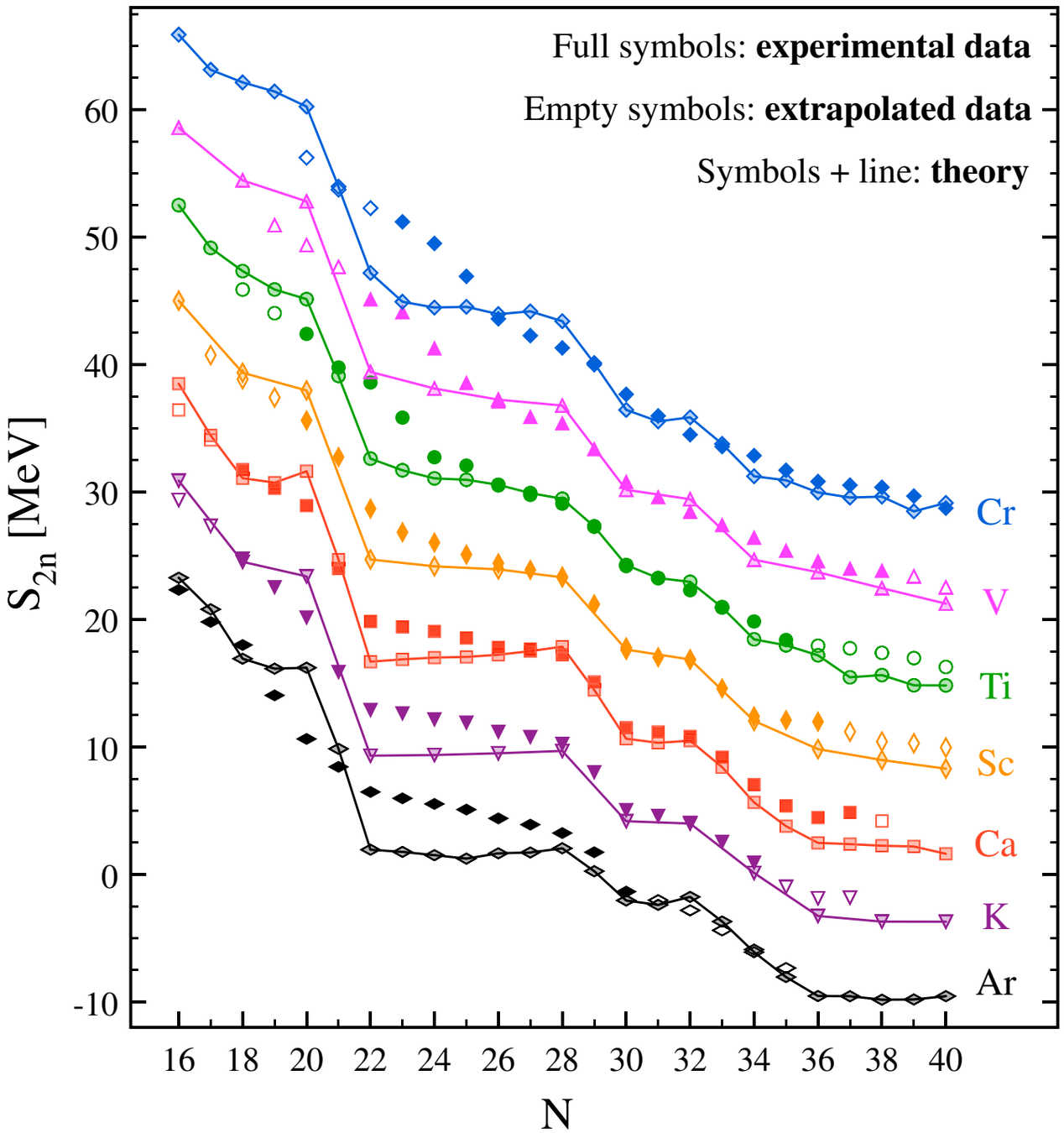
- **Generalises GFs to U(1) breaking**
  - Normal + anomalous propagators
  - First symmetry-breaking ab initio method

- **Application to isotopic chains (Z=18-24)**
  - $Z = 20$ (calcium): magic number
  - Above and below: doubly open shells

- **Binding energies**
  - Systematic calculations possible
  - Underbinding corrected at ADC(3) level

[Somà *et al.* 2021]

Gorkov Green's function theory



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- **Application to isotopic chains (Z=18-24)**
  - $Z = 20$ (calcium): magic number
  - Above and below: doubly open shells

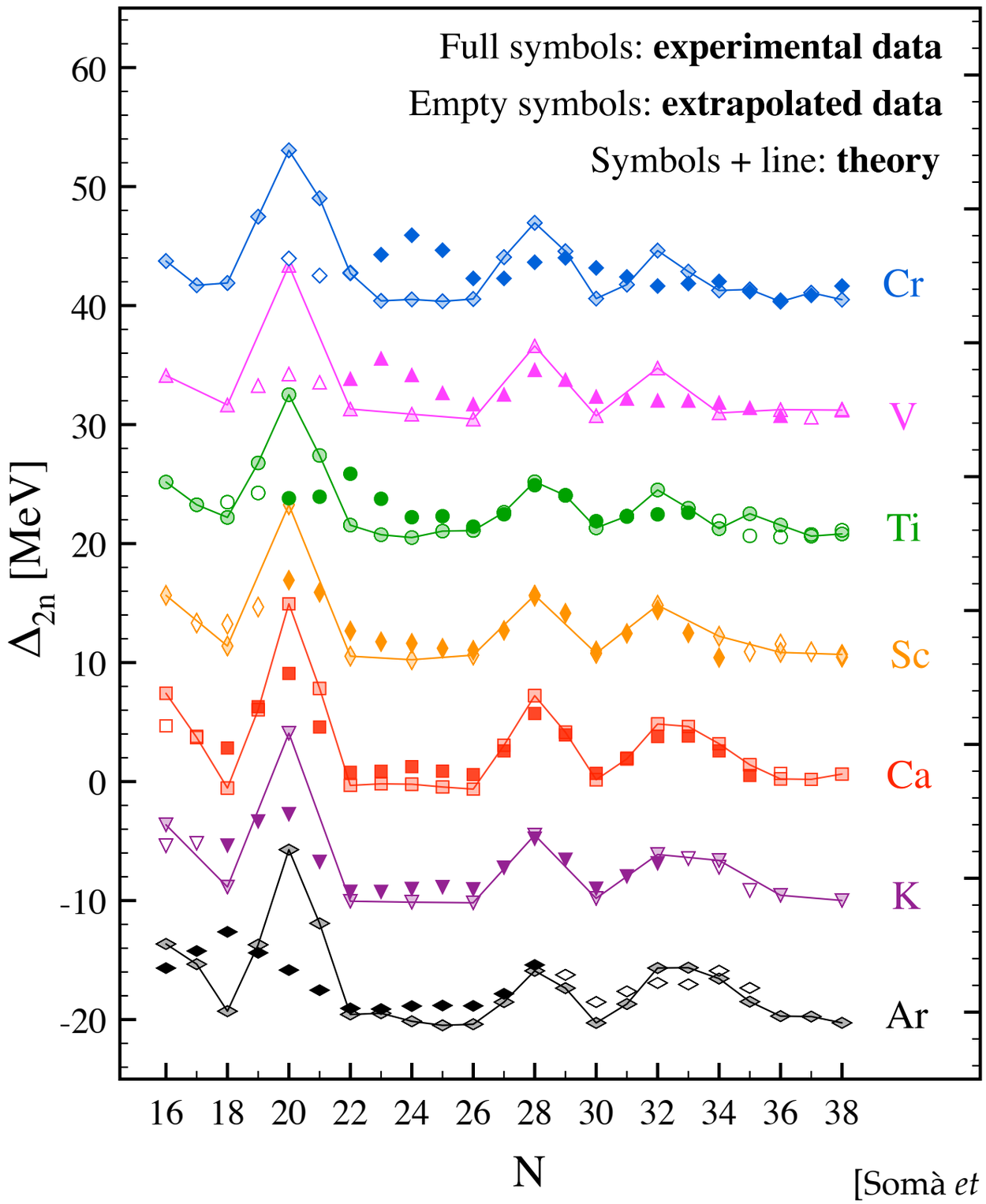
- **Two-neutron separation energies**

$$S_{2n}(N, Z) \equiv |E(N, Z)| - |E(N-2, Z)|$$

  - Error cancellation in relative quantities
  - Drops correspond to magic gaps

[Somà *et al.* 2021]

Gorkov Green's function theory



[Somà *et al.* 2021]

⊙ **Generalises GFs to U(1) breaking**

- ○ Normal + anomalous propagators
- ○ First symmetry-breaking ab initio method

⊙ **Application to isotopic chains (Z=18-24)**

- ○ $Z = 20$ (calcium): magic number
- ○ Above and below: doubly open shells

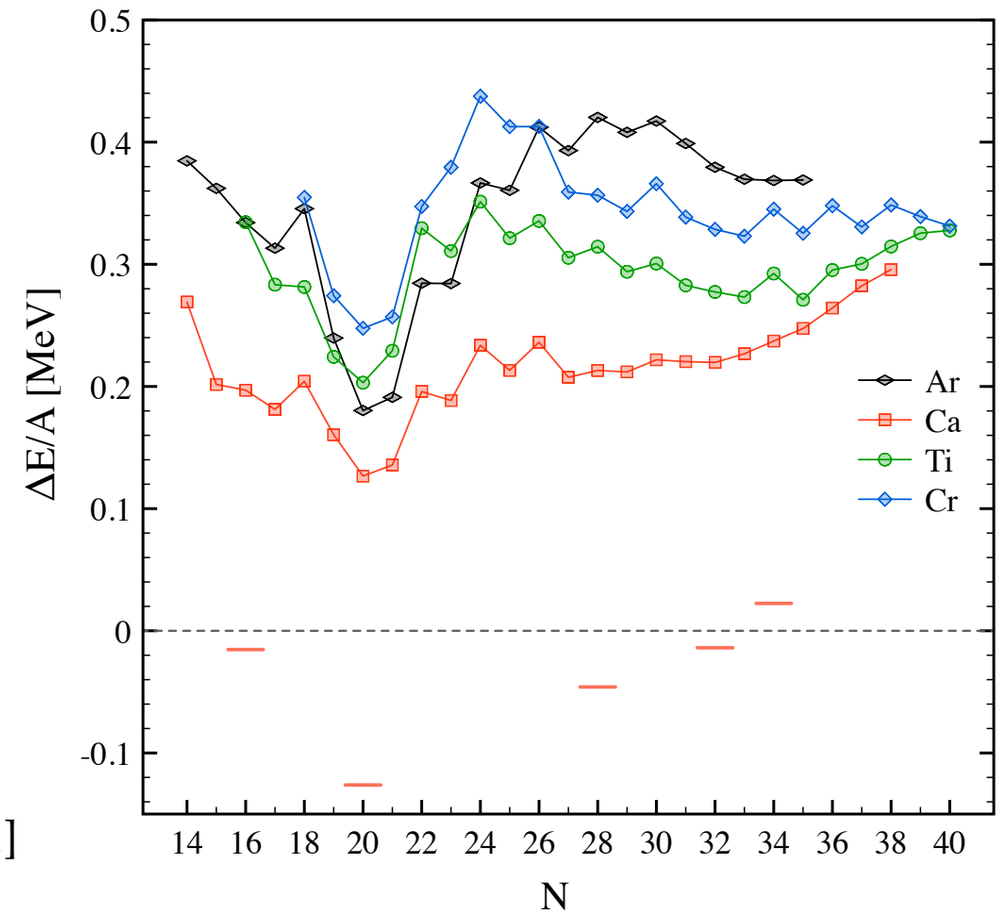
⊙ **Two-neutron shell gaps**

$$\Delta_{2n}(N,Z) \equiv S_{2n}(N,Z) - S_{2n}(N+2,Z)$$

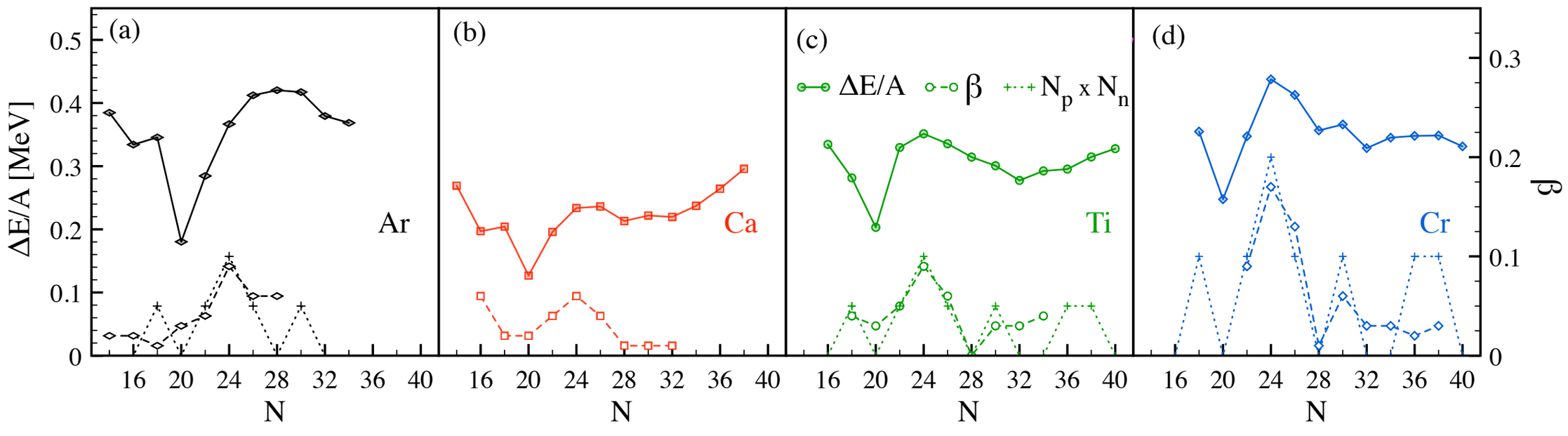
- ○ Measure of ph gap
- ○ **Magic numbers emerge *ab initio*!**
- ○ $N = 20$ gap too large
- ○ Agreement deteriorates away from calcium

Gorkov Green's function theory

- **Energy per nucleon: theory vs. experiment**
  - Well-defined minimum at magic $N = 20$
  - Correlation with measures of deformation
  - Calls for breaking of SU(2)

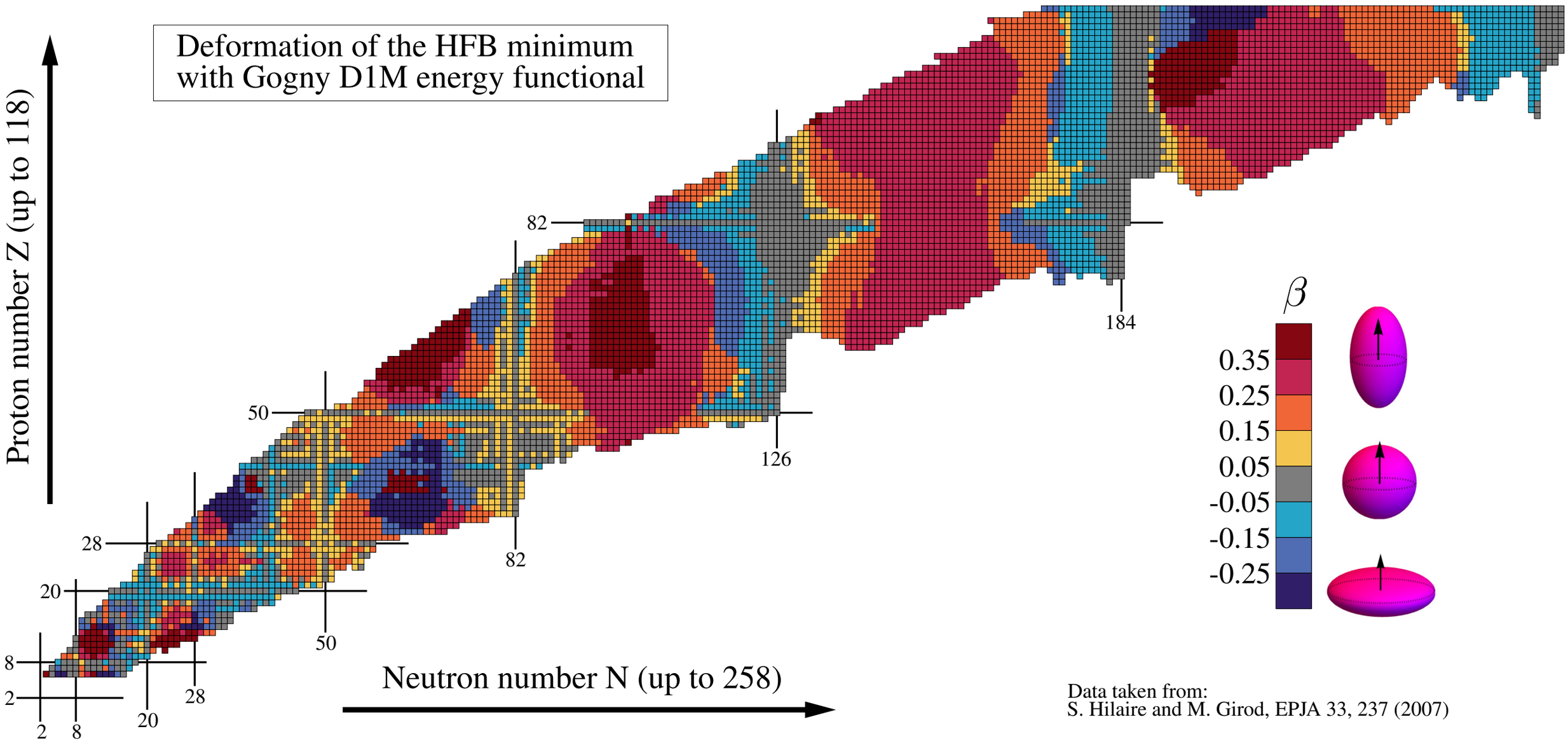


[Somà *et al.* 2021]



Deformation across the nuclear chart

[*Figure:* B. Bally]



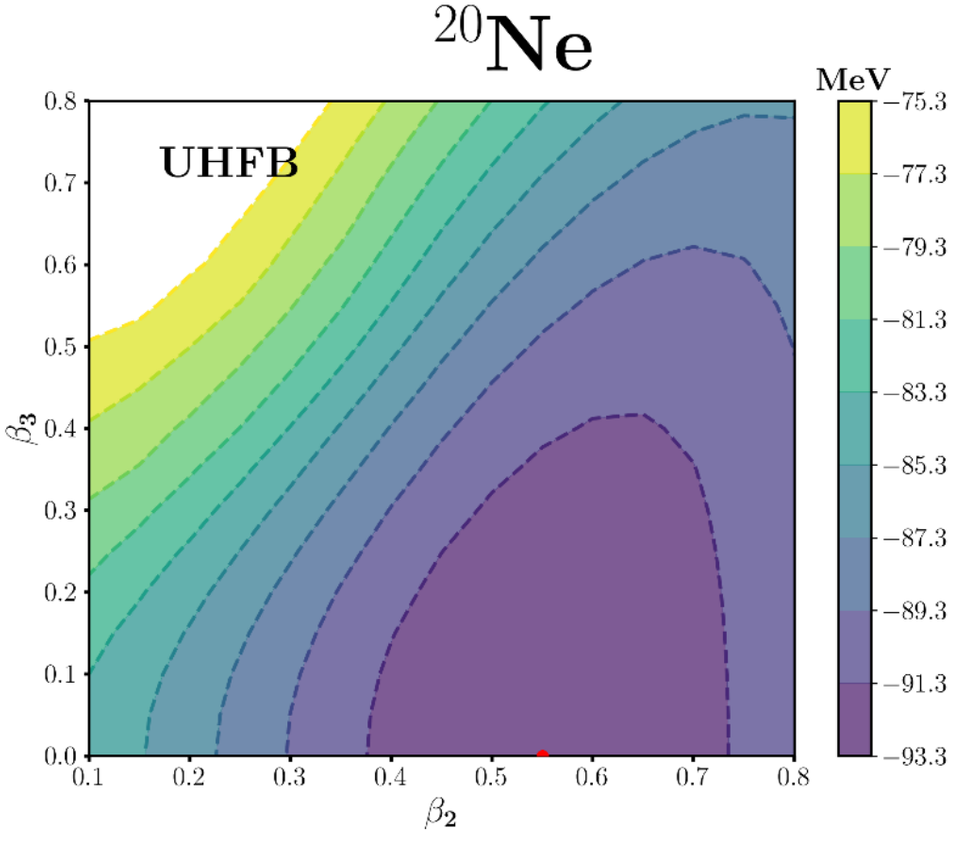
Data taken from:
S. Hilaire and M. Girod, EPJA 33, 237 (2007)

➪ Majority of nuclei display a non-spherical mean field (when allowed to do so)

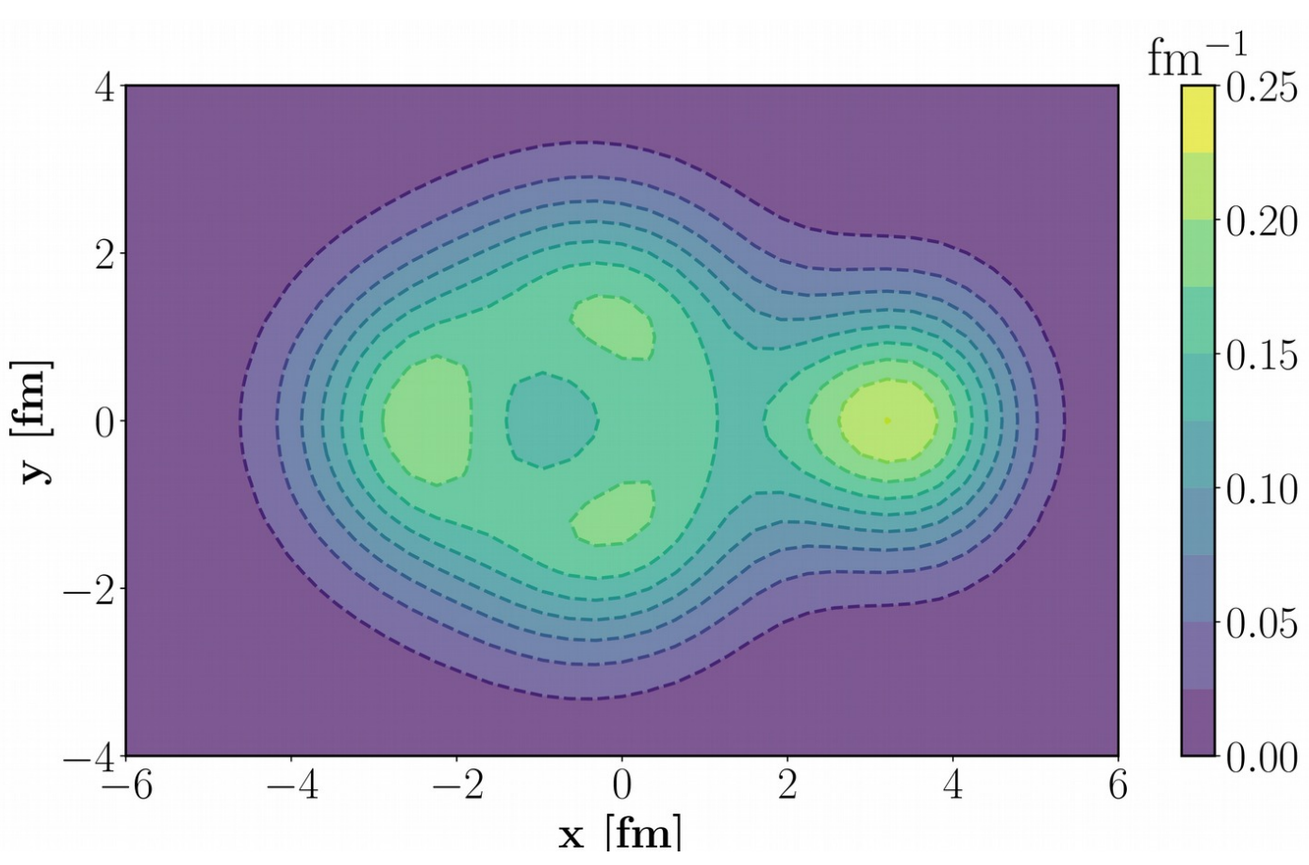
Breaking SU(2)

- **Ongoing efforts to extend state-of-the-art techniques to SU(2)-breaking**
  - Coupled cluster: only SU(2) → deformed CC
  - MBPT: on top of U(1) → deformed BMBPT

↓ Example from deformed (= unrestricted) HFB [Frosini *et al.* in preparation]



Energy surface

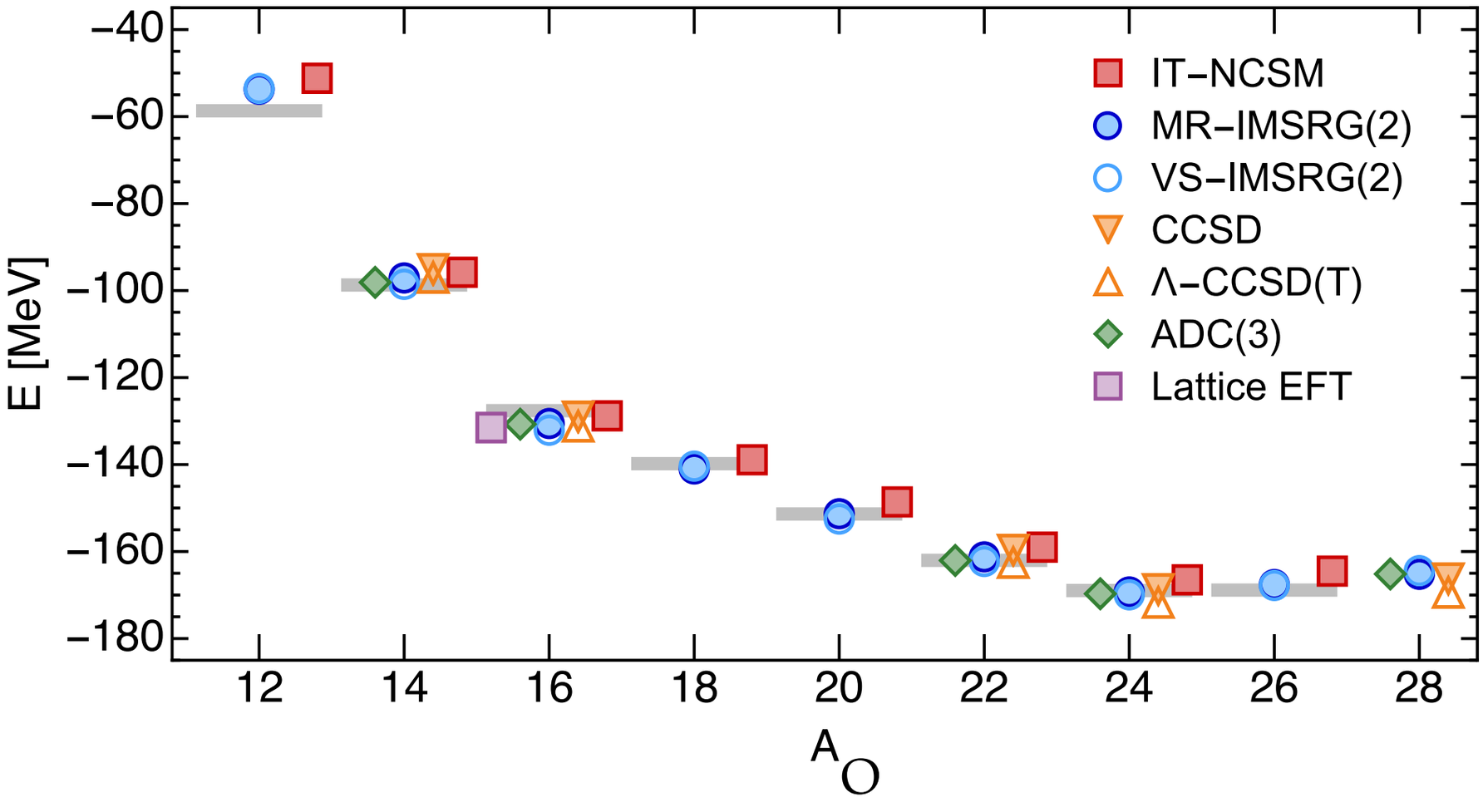


Matter density

Contents

Benchmarking many-body approaches

- **Different many-body calculations yield very consistent results**
  - All within few %
  - MBPT not shown but wouldn't be too far
  - Discrepancies w.r.t. data to be **attributed to the input Hamiltonian**

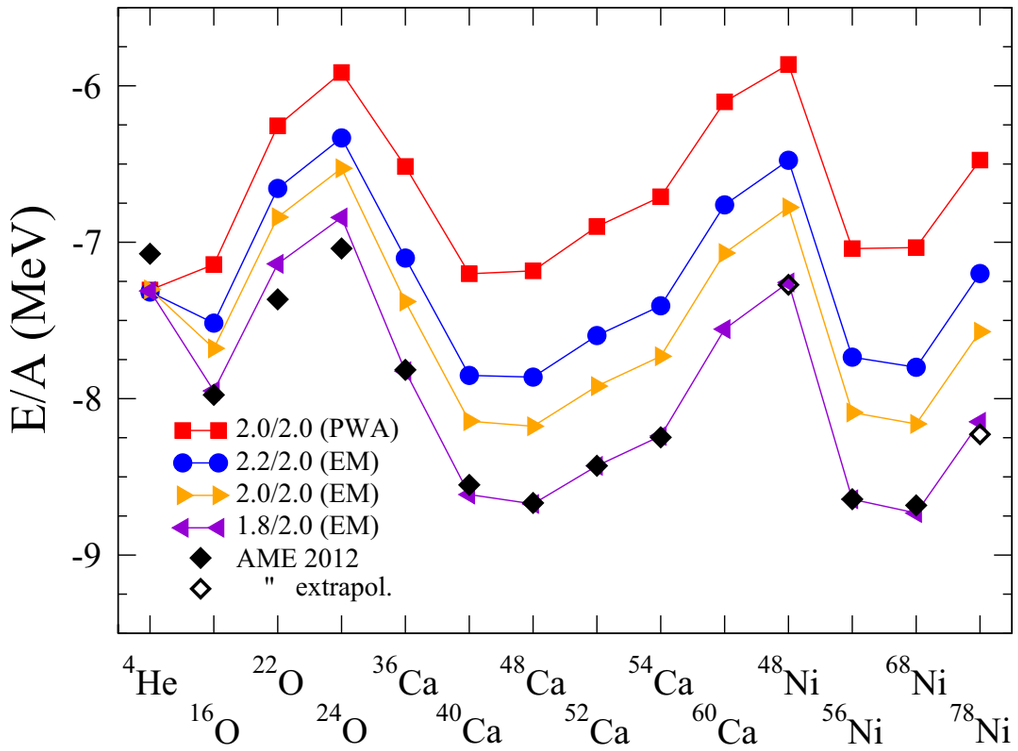


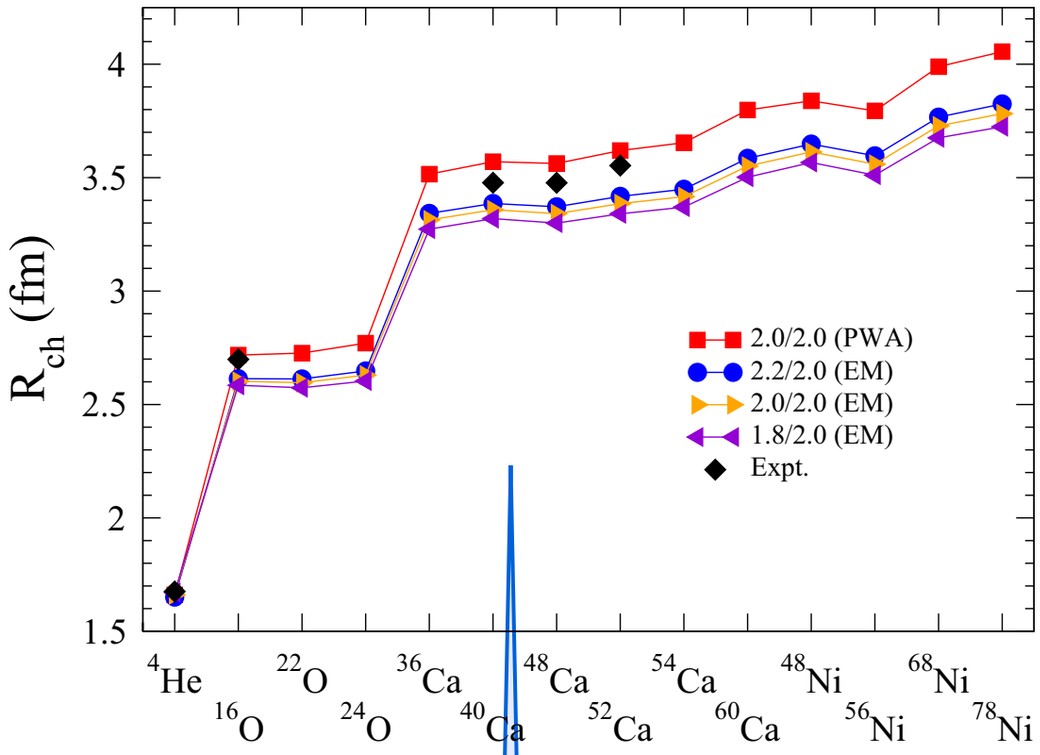
[Hergert 2020]

Proliferation of nuclear Hamiltonians

- **State of the art (until very recently)**
  - No routine/consistent account of systematic uncertainties coming from input Hamiltonian
  - Precision ultimately depends on the chosen input
  - Proliferation of Hamiltonians

[Simonis *et al.* 2017]



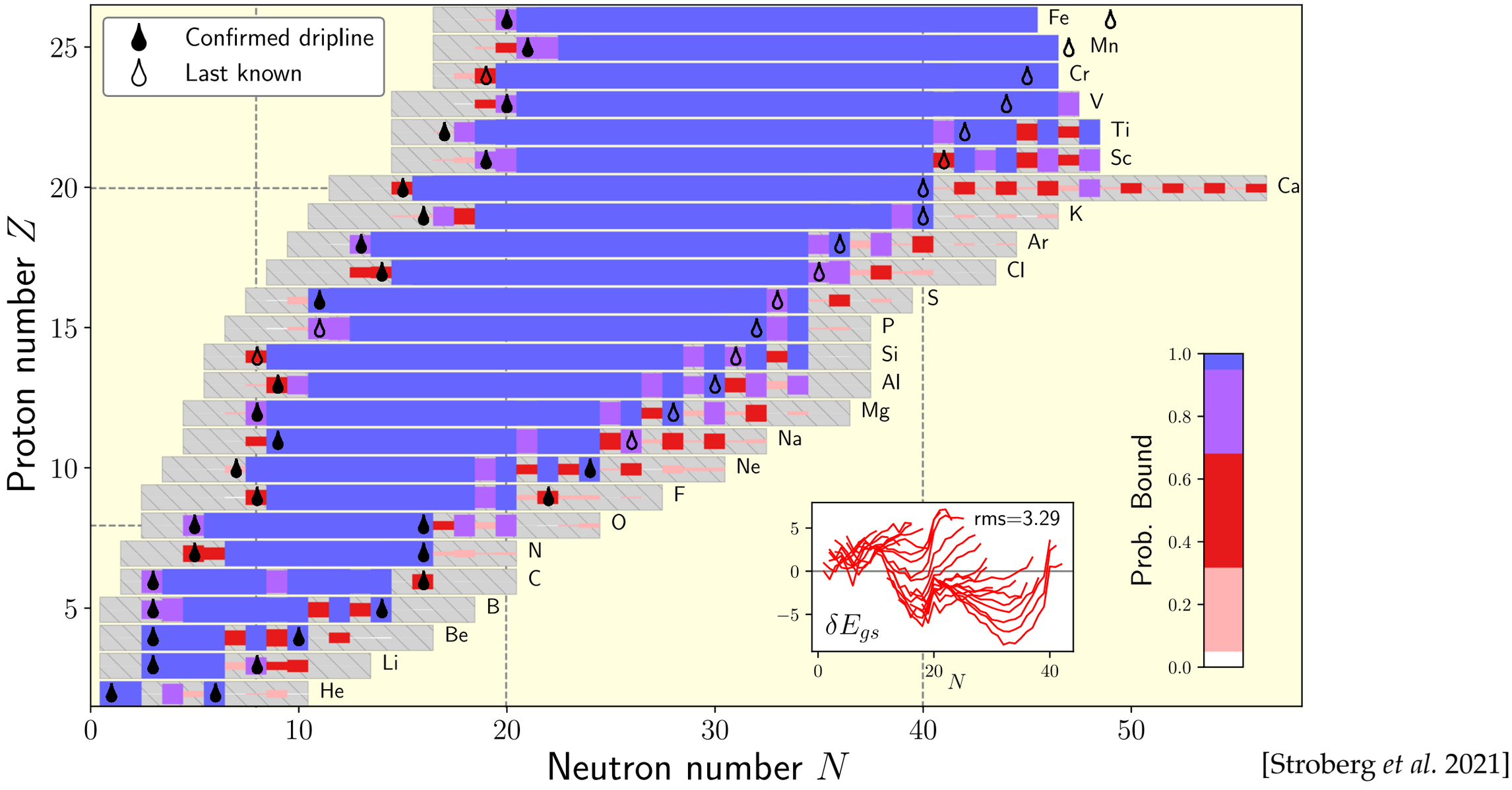


- **Need to correctly describe nuclear sizes prompted changes in fitting procedures**
  - Mid-mass observables included in the fit of LECs
  - Compromise accuracy on NN data, few-body & spectroscopy

→ **NNLO$_{sat}$**

Ab initio prediction of the drip lines

- **Systematic survey of light and medium-mass nuclei** (method: valence-space IMSRG)
  - Good description (+ prediction) of proton and neutron drip lines
  - **Rms deviation** on total binding energies = **3.3 MeV** (cf. **0.7 MeV** in energy density functionals)



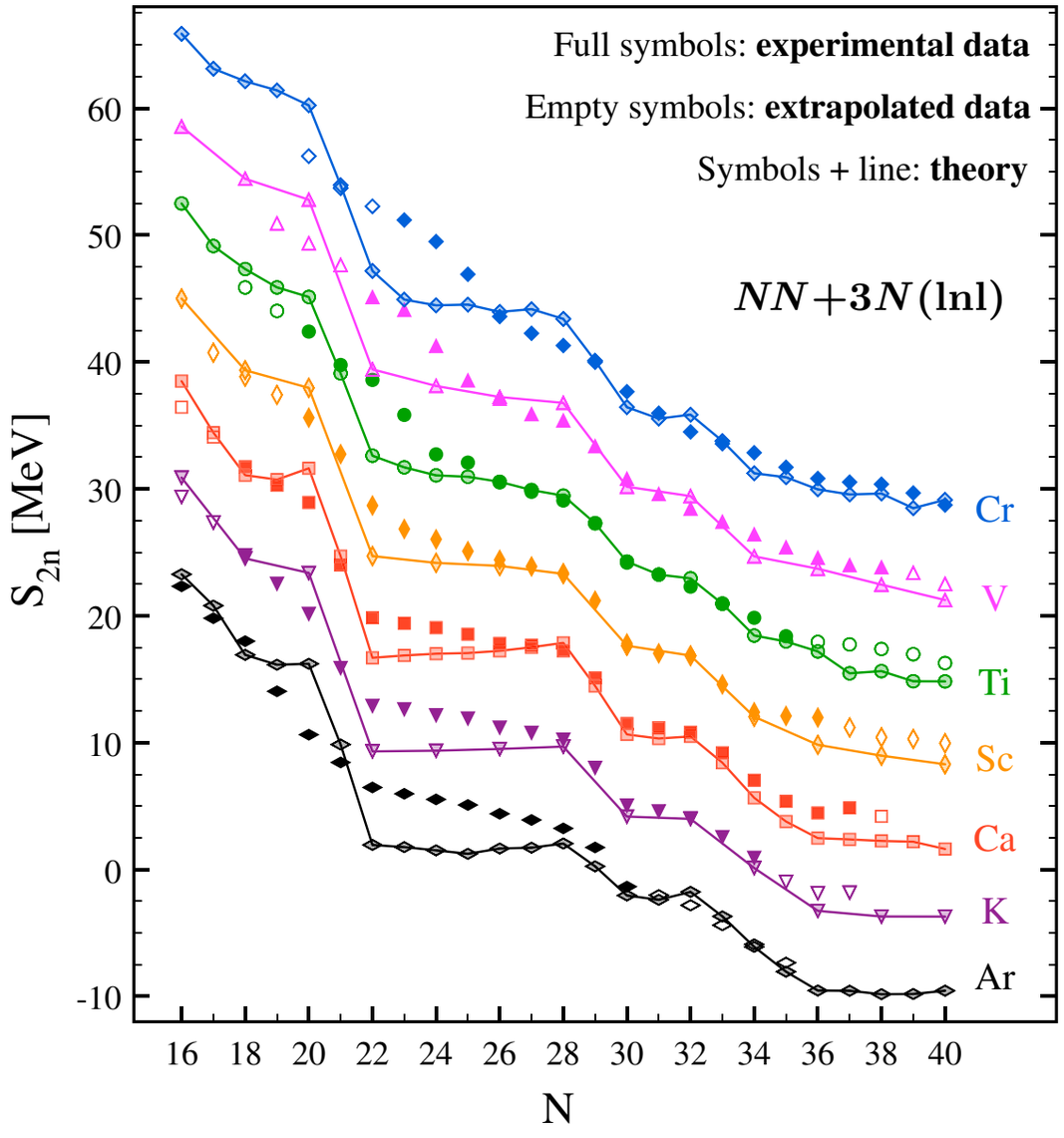
[Stroberg *et al.* 2021]

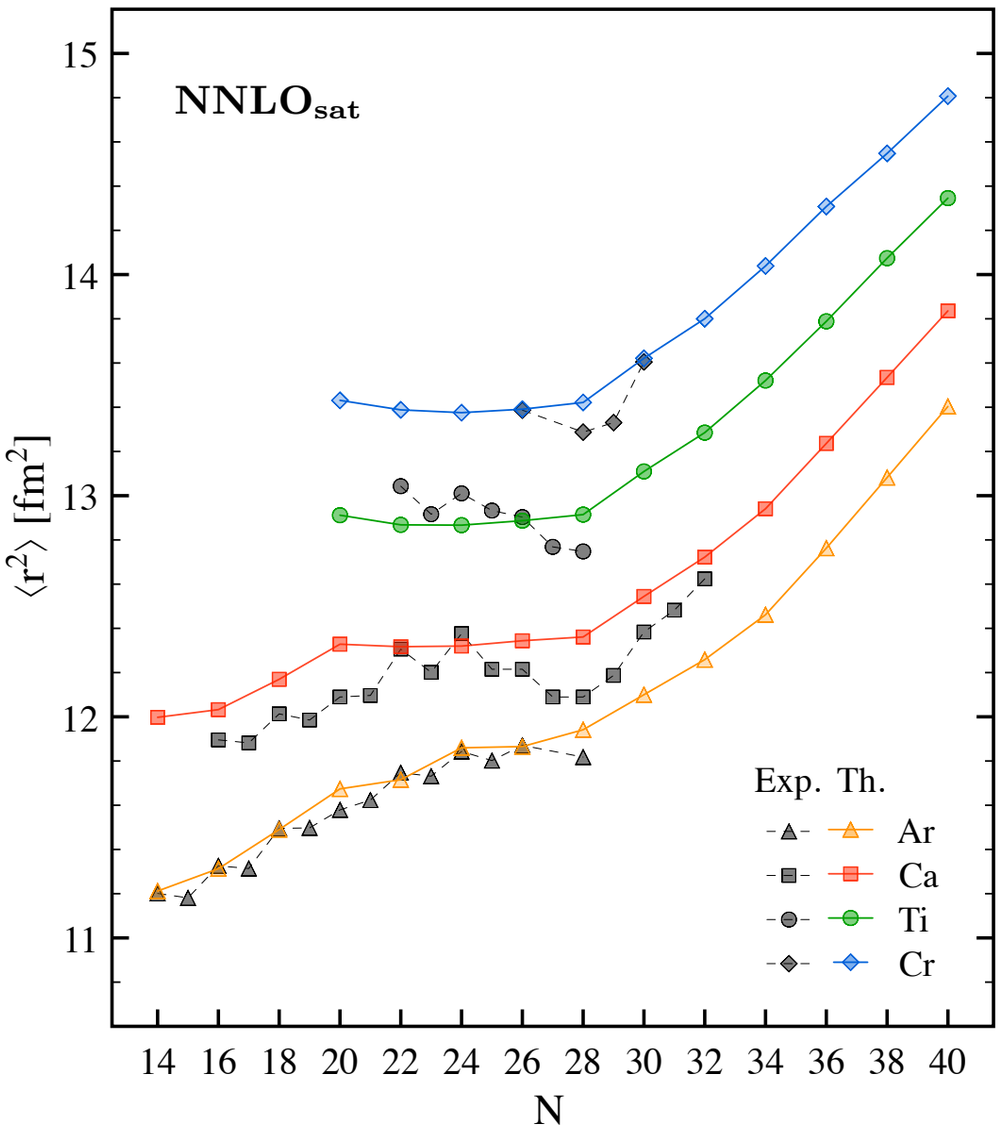
Mid-mass isotopic chains

- **SCGF calculations along mid-mass chains**
  - ADC(2) level: few % on differential quantities
  - ADC(3) level: 2.5 % on B.E. of closed-shells
  - Radii within few % but some features are missing

Gorkov ADC(2) [Somà *et al.* 2021]

	Ar	Ca	Ti	Cr
$\boldsymbol{NN+3N}$**(lnl)**				
E [MeV]	14.1	10.3	14.2	19.2
E/A [MeV]	0.34	0.21	0.29	0.35
S_{2n} [MeV]	2.90	1.56	2.05	2.22
NNLO$_{\mathbf{sat}}$				
$\langle r^2_{\rm ch}\rangle^{1/2}$ [fm]	0.008	0.022	0.019	0.010
$\delta\langle r^2_{\rm ch}\rangle^{1/2}$ [fm]	0.008	0.024	0.023	0.013

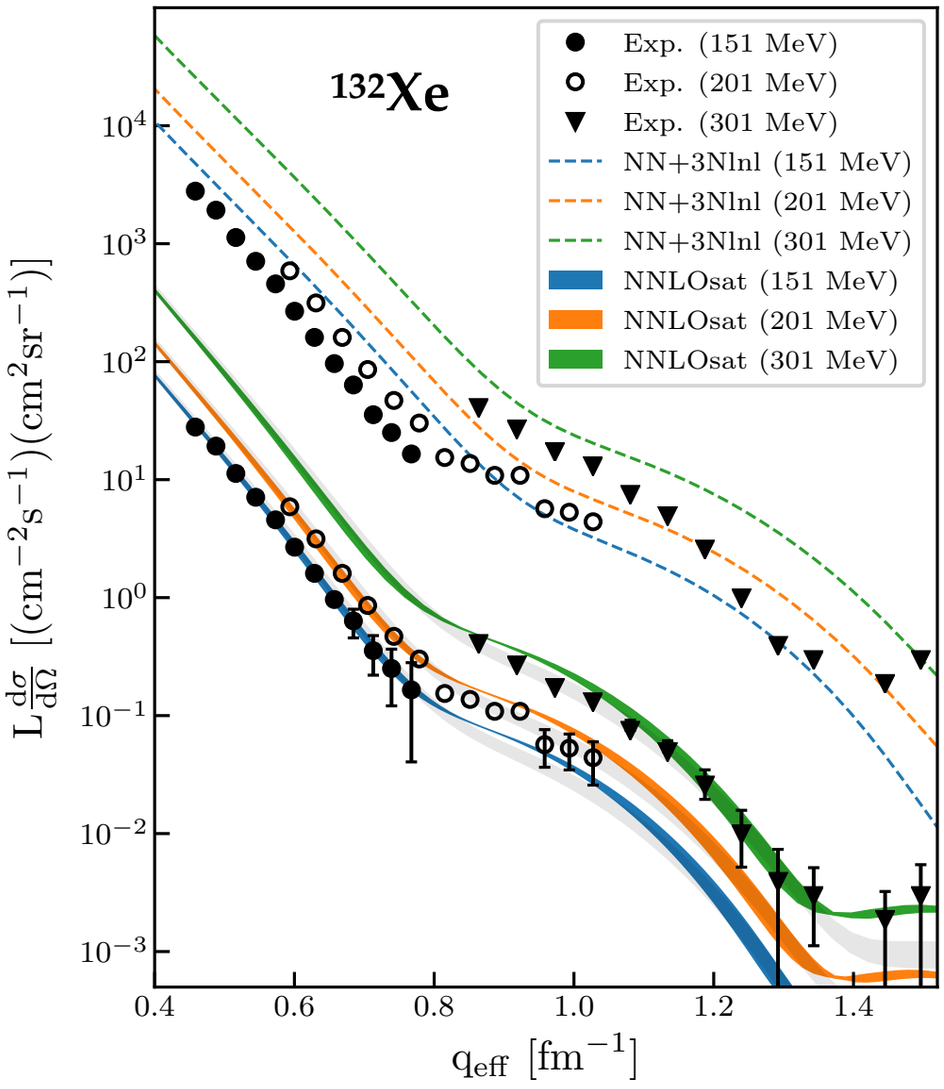




Electron scattering cross sections

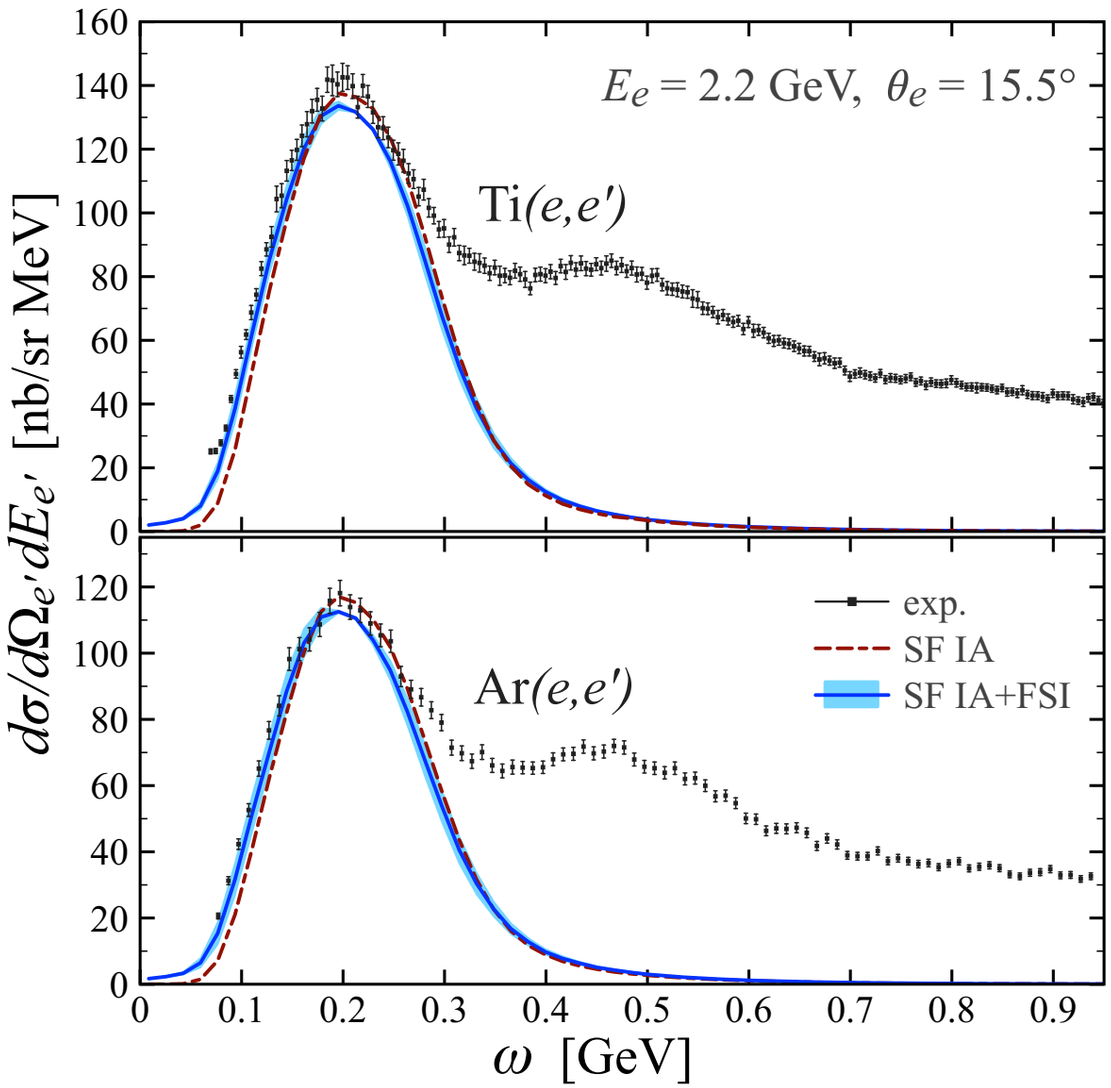
- **Correct reproduction of radii crucial when computing cross sections**
  - Particularly important for nuclear physics applications to other domains

Elastic electron scattering @SCRIT



[Arthuis *et al.* 2020]

Inelastic electron scattering @JLAB



[Barbieri *et al.* 2019]

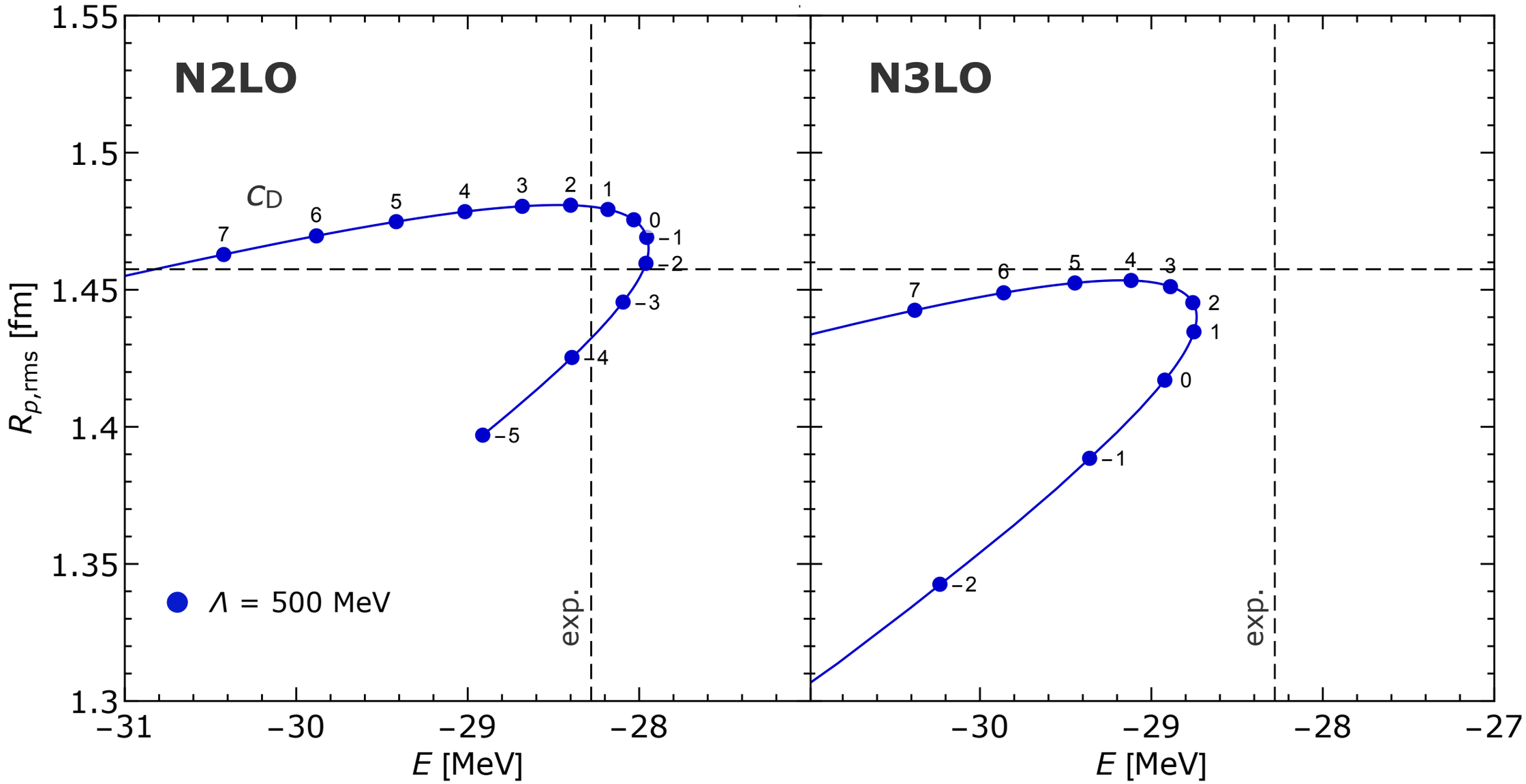
Systematic fit of low-energy constants

⊙ **Example of fit of low-energy constants (LECs) in the three-body sector**

○ Two LECs (c_D & c_E) at N^{2}LO and N^{3}LO

○ $\mathbf{c_D}$ as a parameter in the calculation of E(^{4}He) & r(^{4}He), $\mathbf{c_E}$ determined to reproduce E(^{3}H)

[Hüther *et al.* 2020]



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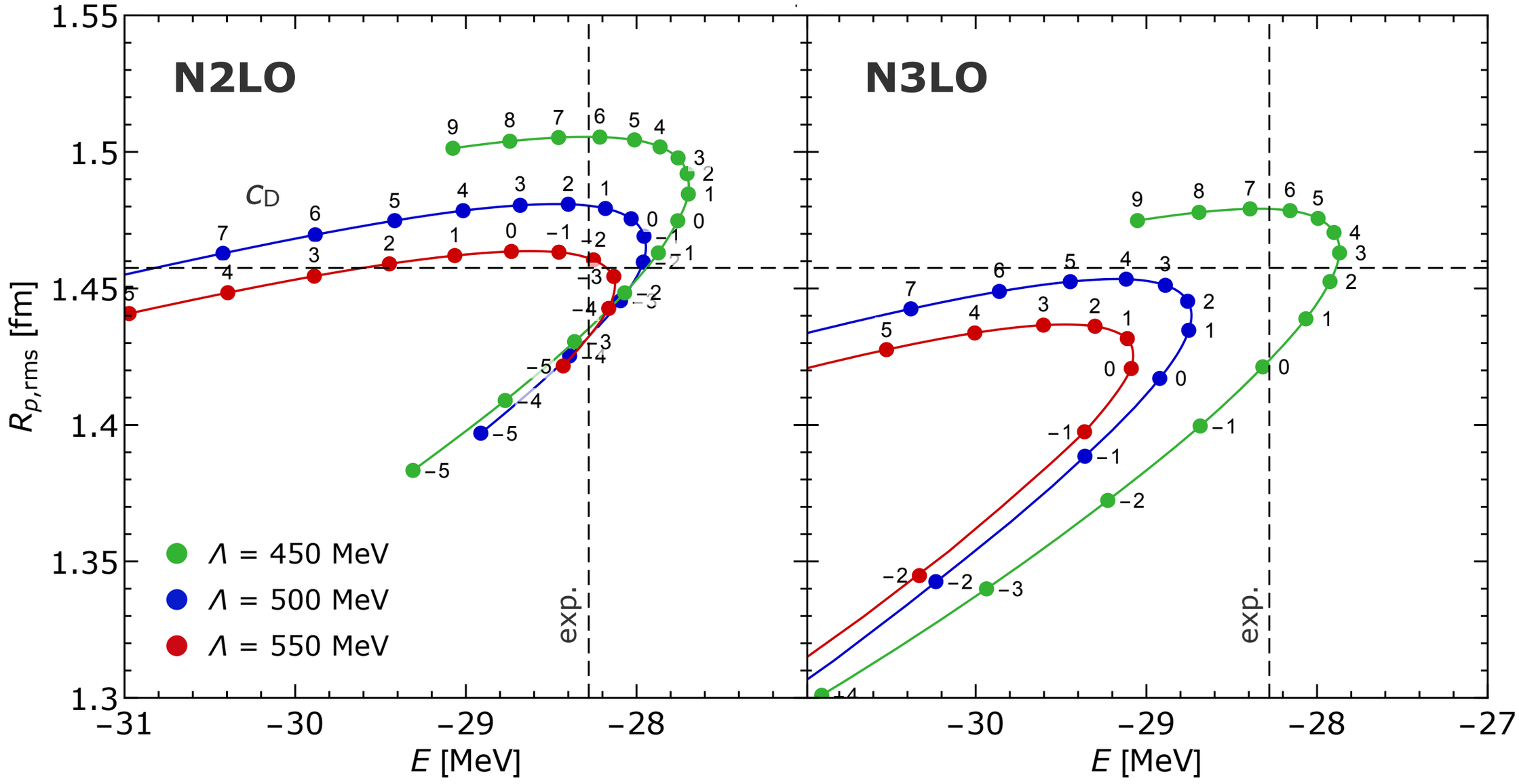
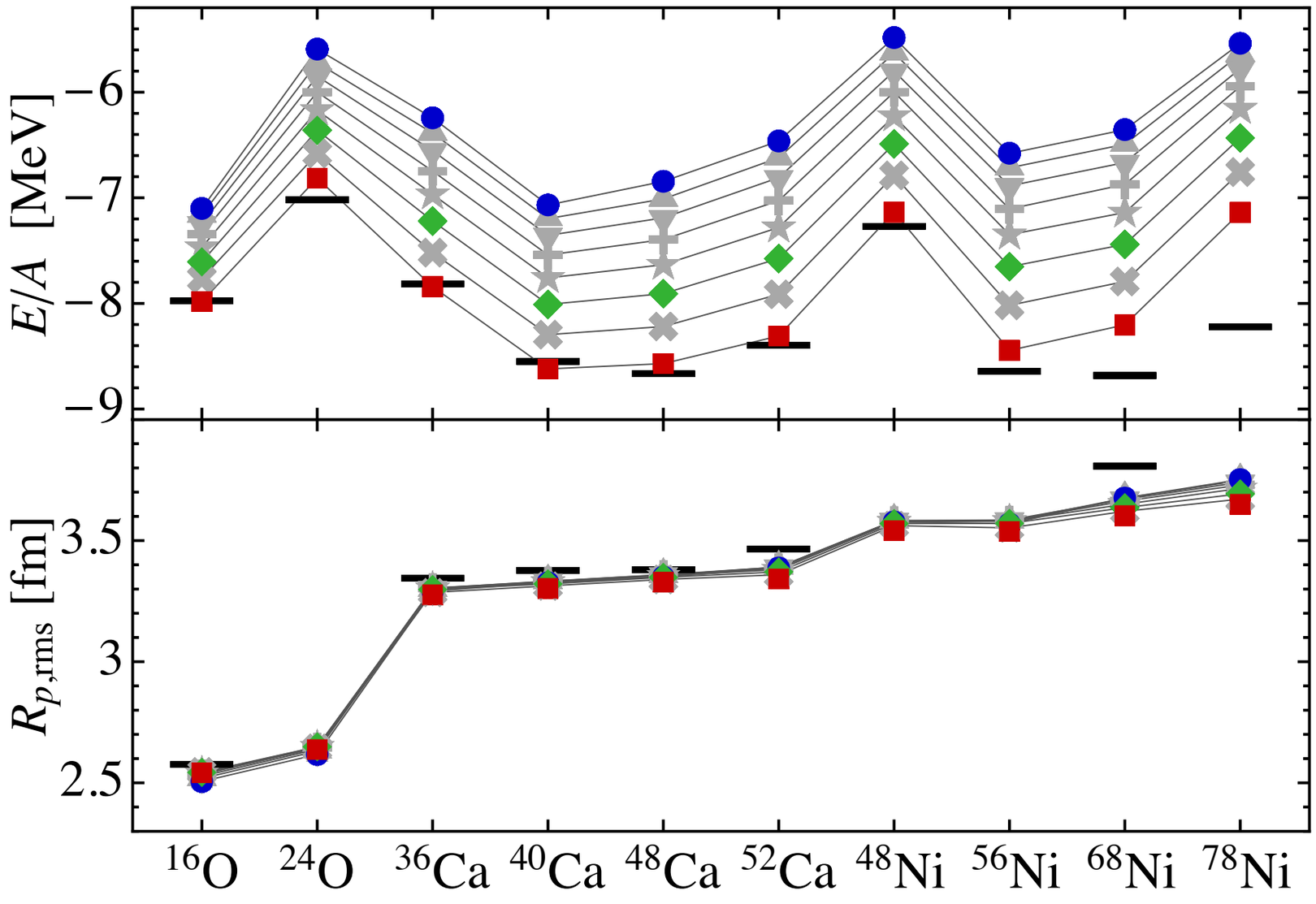
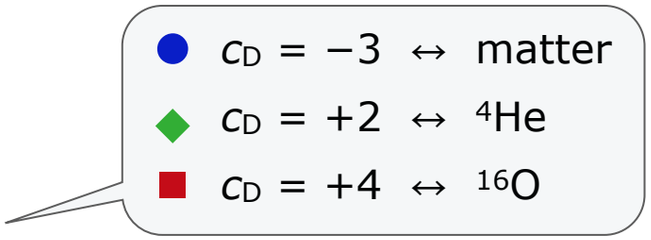


Application to medium-mass nuclei





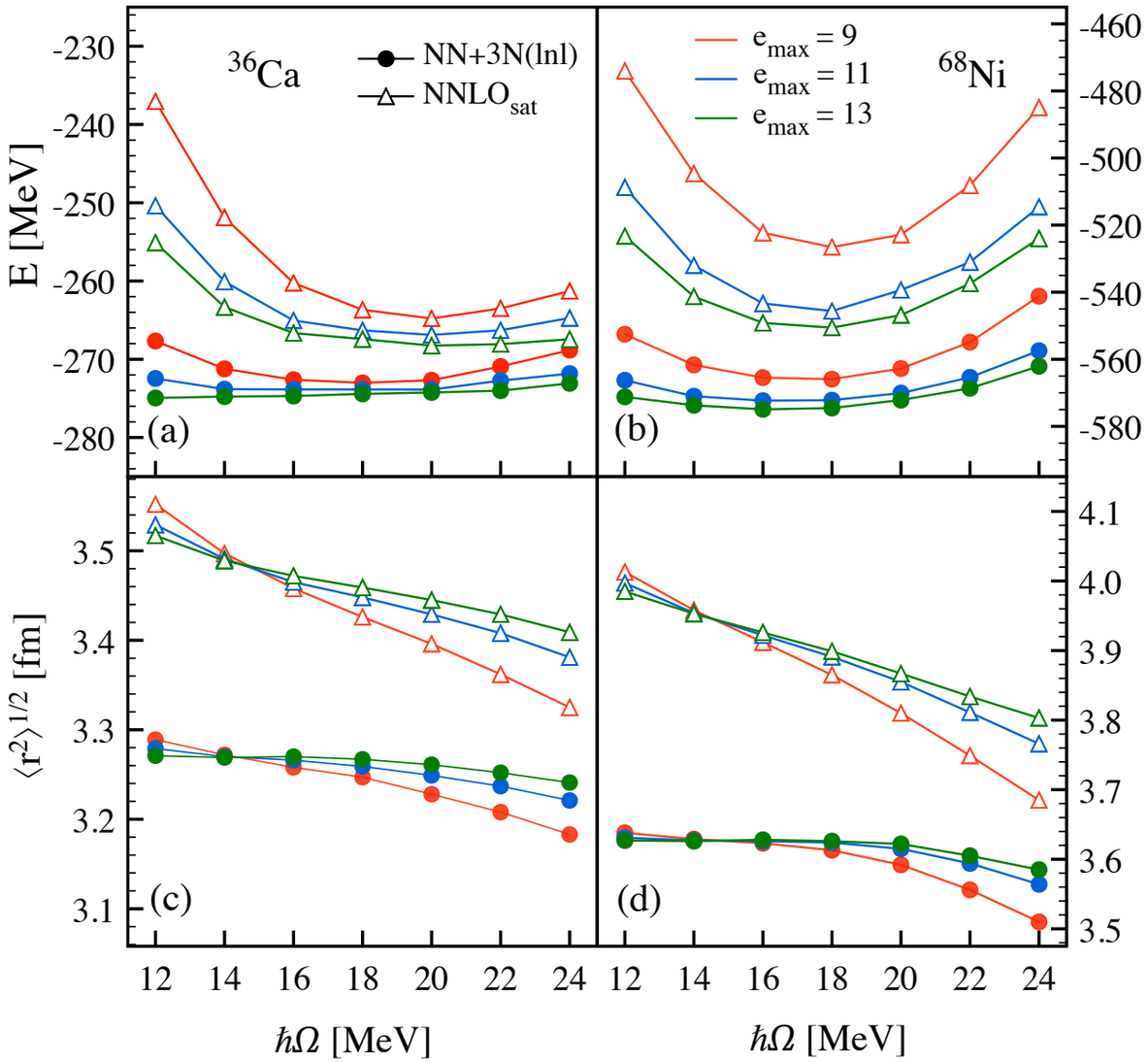
N3LO
$\Lambda = 500$ MeV

[Hüther *et al.* 2020]

- Large sensitivity to 3N parameters
- **"Tension" between optimal values in few-body systems, mid-mass nuclei & nuclear matter**
- Radii not much affected by changes in c_D & c_E (regulator more important)

Assessing uncertainties

- **Uncertainties from the expansion method**
  - Basis truncation



[Soma *et al.* 2020]

Assessing uncertainties

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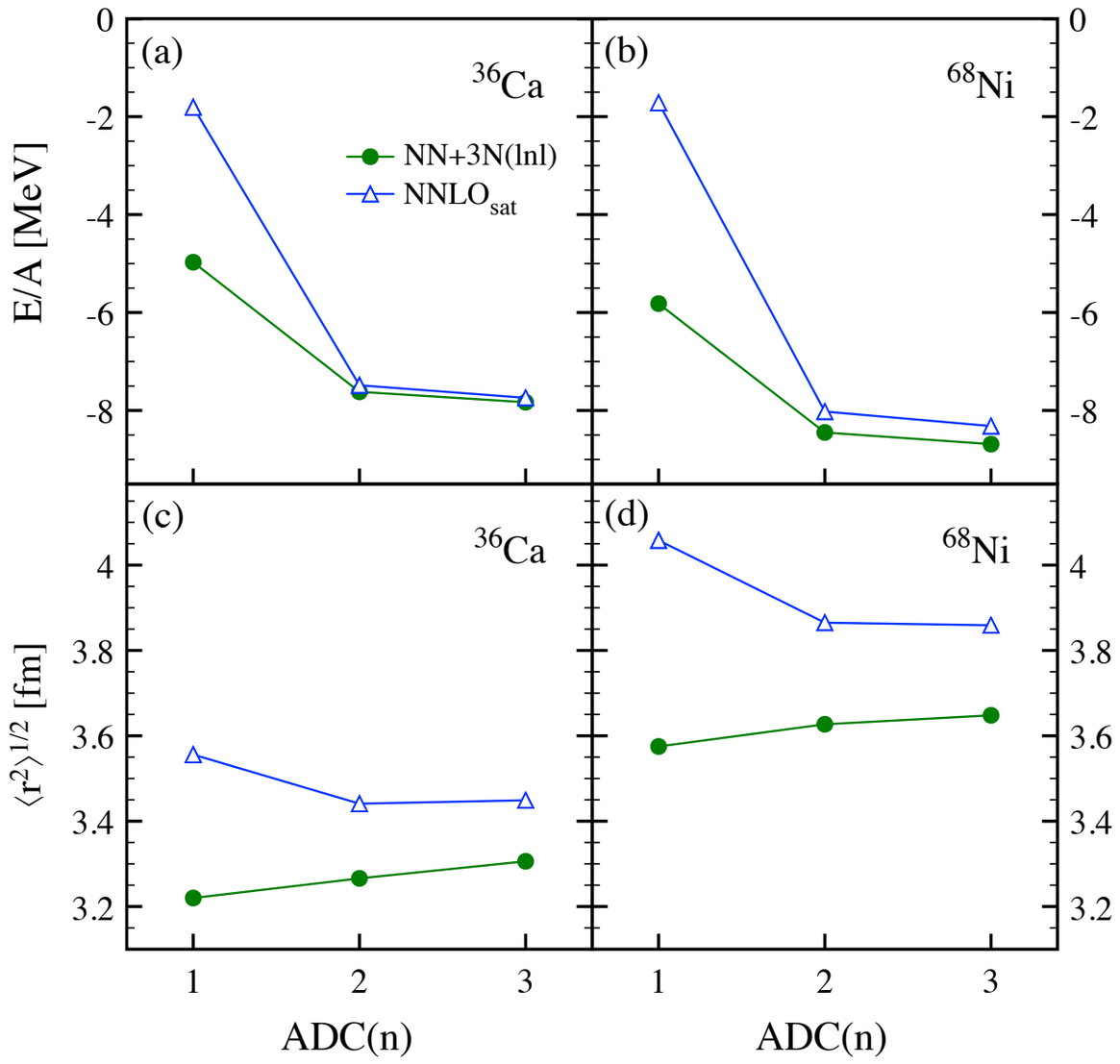
  - Many-body truncation



[Soma *et al.* 2020]

Assessing uncertainties

- **Uncertainties from the expansion method**
  - Basis truncation
  - Many-body truncation
  - Symmetry breaking (if any)
  - Neglected induced operators (if any)
  - …

[Soma *et al.* 2021]	NN+3N(lnl)		$\mathrm{NNLO_{sat}}$
	E	r_{ch}	r_{ch}
Model space (e_{max})	0.5%	$< 0.1\%$	0.5%
Model space ($e_{3\mathrm{max}}$)	0.2%	0.2%	0.3%
ADC truncation	2%	0.5%	$< 0.1\%$
U(1) breaking	0.2%	$< 0.1\%$	$< 0.1\%$
Neglected induced op.	2%	1%	–
Total	2.9%	1.1%	0.6%

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⊙ **Uncertainties from the Hamiltonian**

- ○ Ideally, at each order from cutoff variation
- ○ If not possible, use some estimate

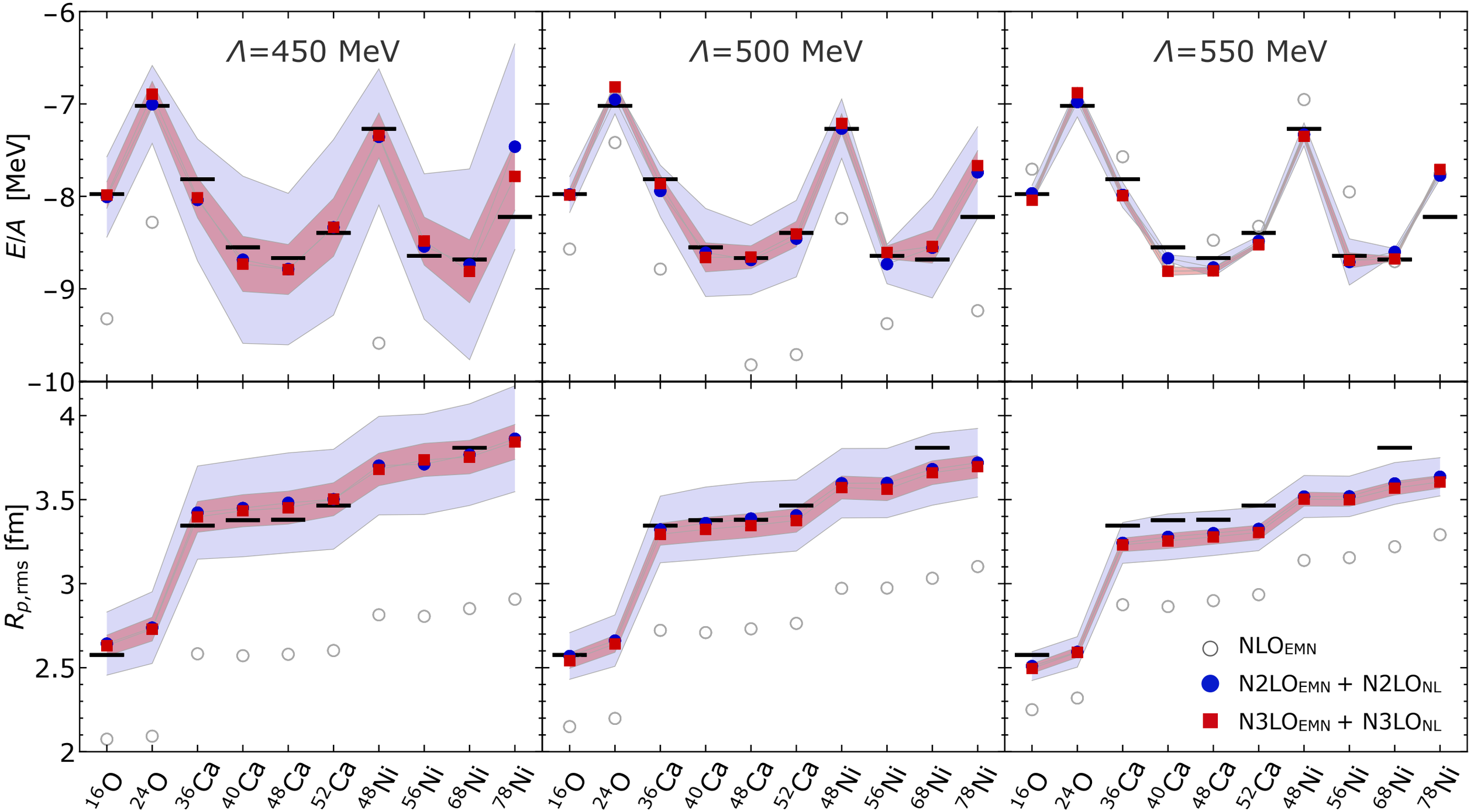
[Epelbaum *et al.* 2015]

$$\Delta X^{\mathrm{N^3LO}}(p) = \max\left(Q^5 \times \left|X^{\mathrm{LO}}(p)\right|,\quad Q^3 \times \left|X^{\mathrm{LO}}(p) - X^{\mathrm{NLO}}(p)\right|,\quad Q^2 \times \left|X^{\mathrm{NLO}}(p) - X^{\mathrm{N^2LO}}(p)\right|,\right.$$
$$\left. Q \times \left|X^{\mathrm{N^2LO}}(p) - X^{\mathrm{N^3LO}}(p)\right|\right),$$

Towards systematic calculations (with uncertainties)

⊙ **Evaluation of uncertainties from the Hamiltonian**

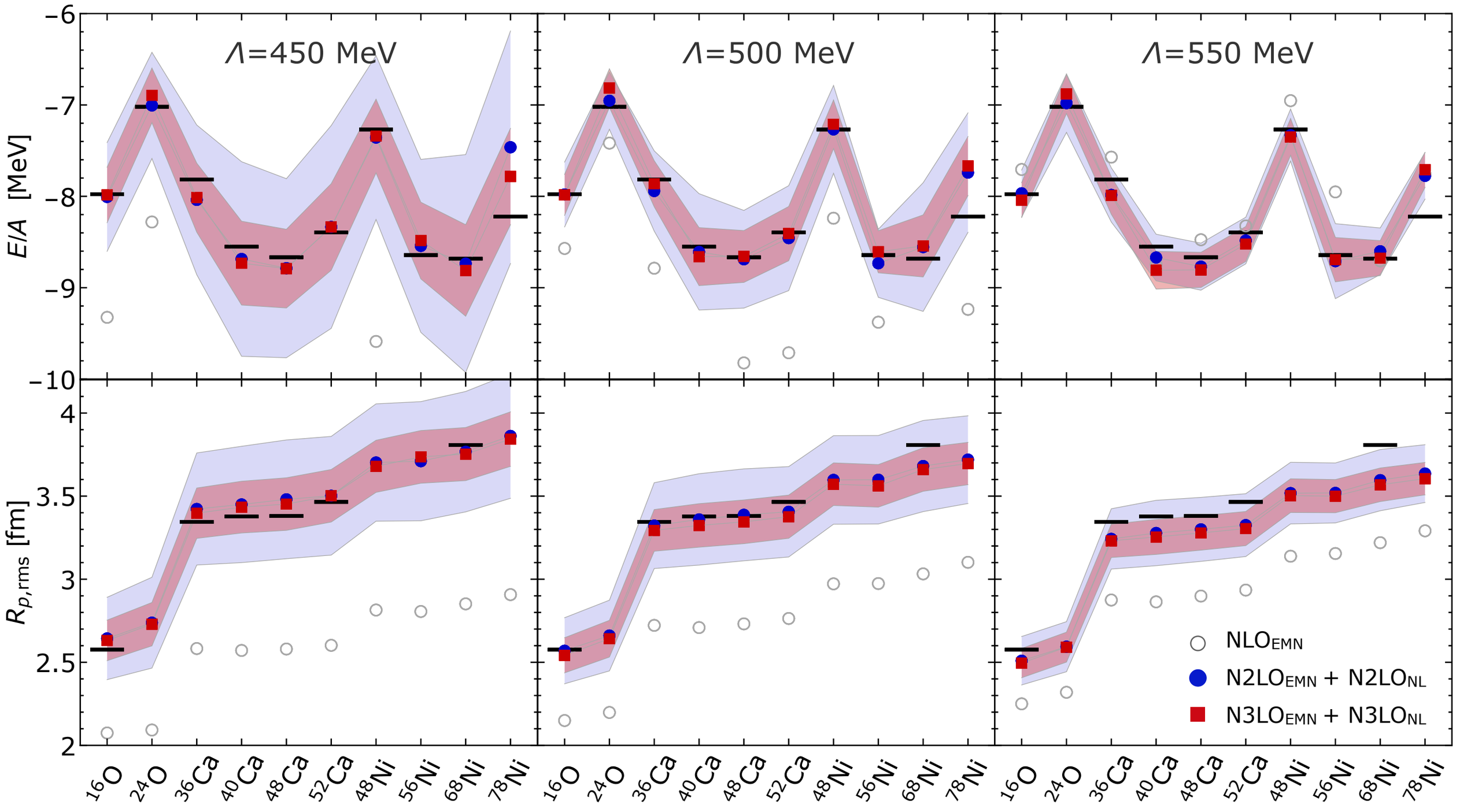
[Hüther *et al.* 2020]



Towards systematic calculations (with uncertainties)

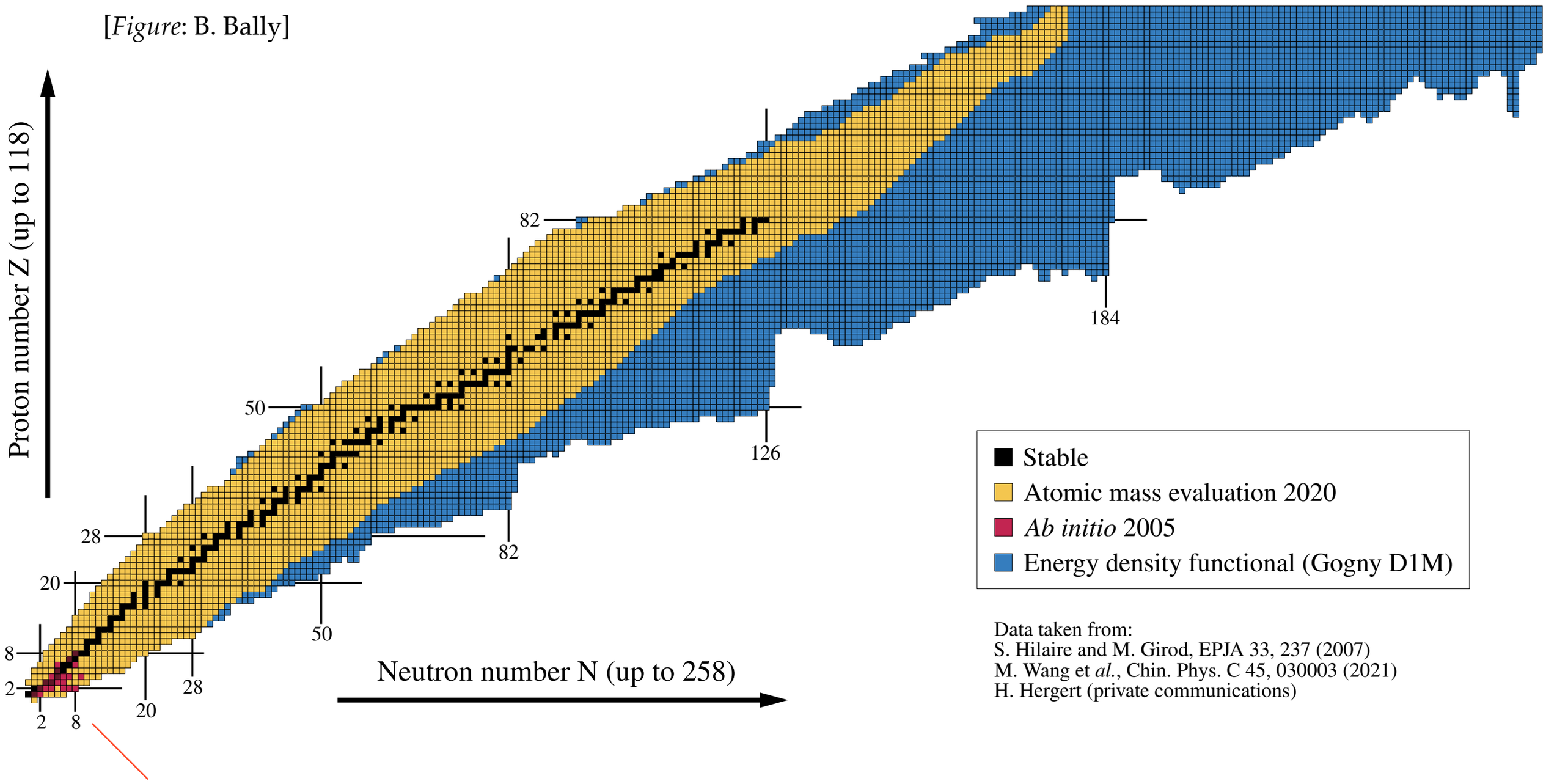
⊙ **Evaluation of uncertainties from the Hamiltonian + the many-body method**

[Hüther *et al.* 2020]



Progress of ab initio calculations

[*Figure*: B. Bally]

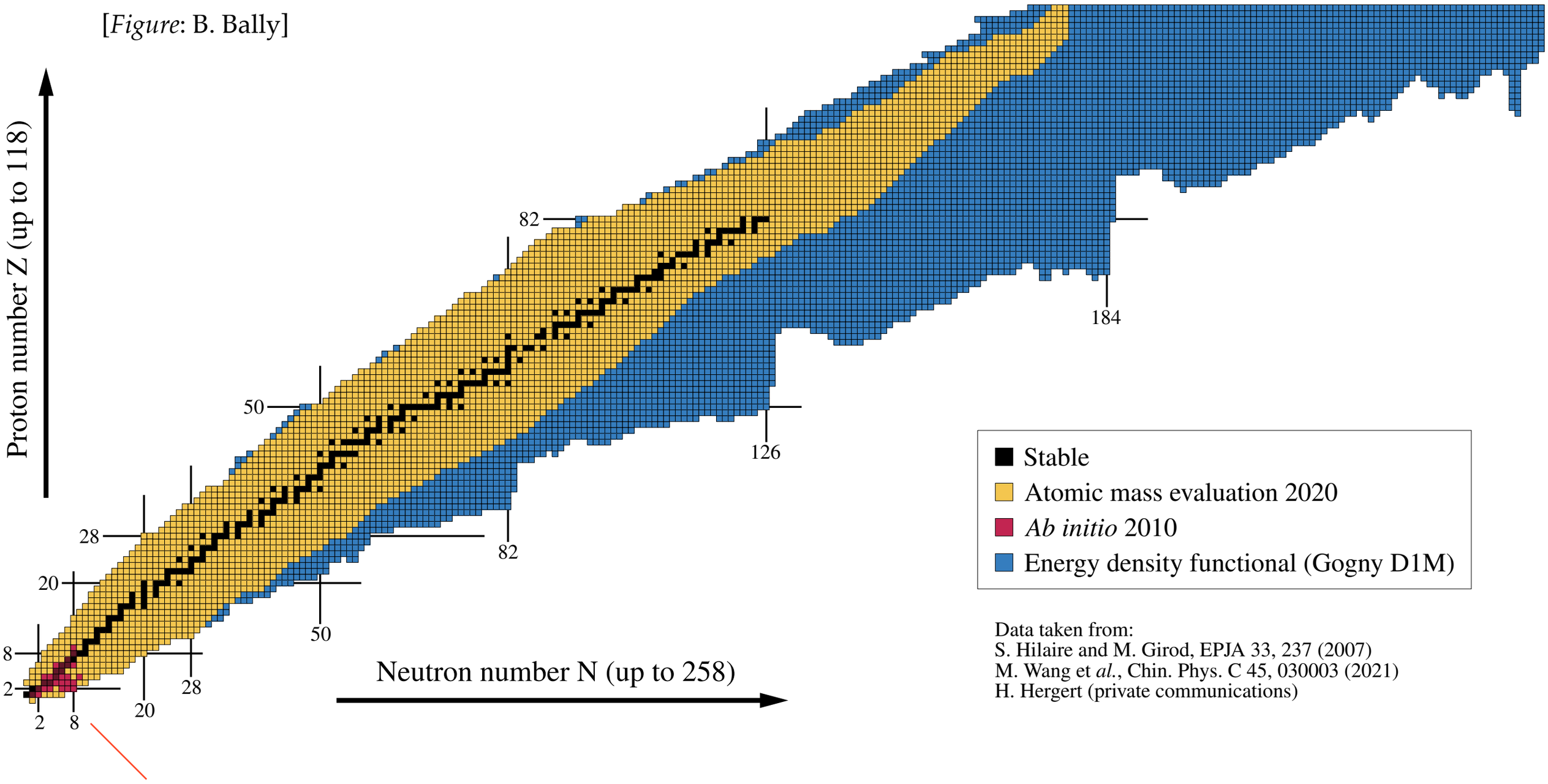


Data taken from:
S. Hilaire and M. Girod, EPJA 33, 237 (2007)
M. Wang et *al.*, Chin. Phys. C 45, 030003 (2021)
H. Hergert (private communications)

- Only exact methods available

Progress of ab initio calculations

[*Figure*: B. Bally]

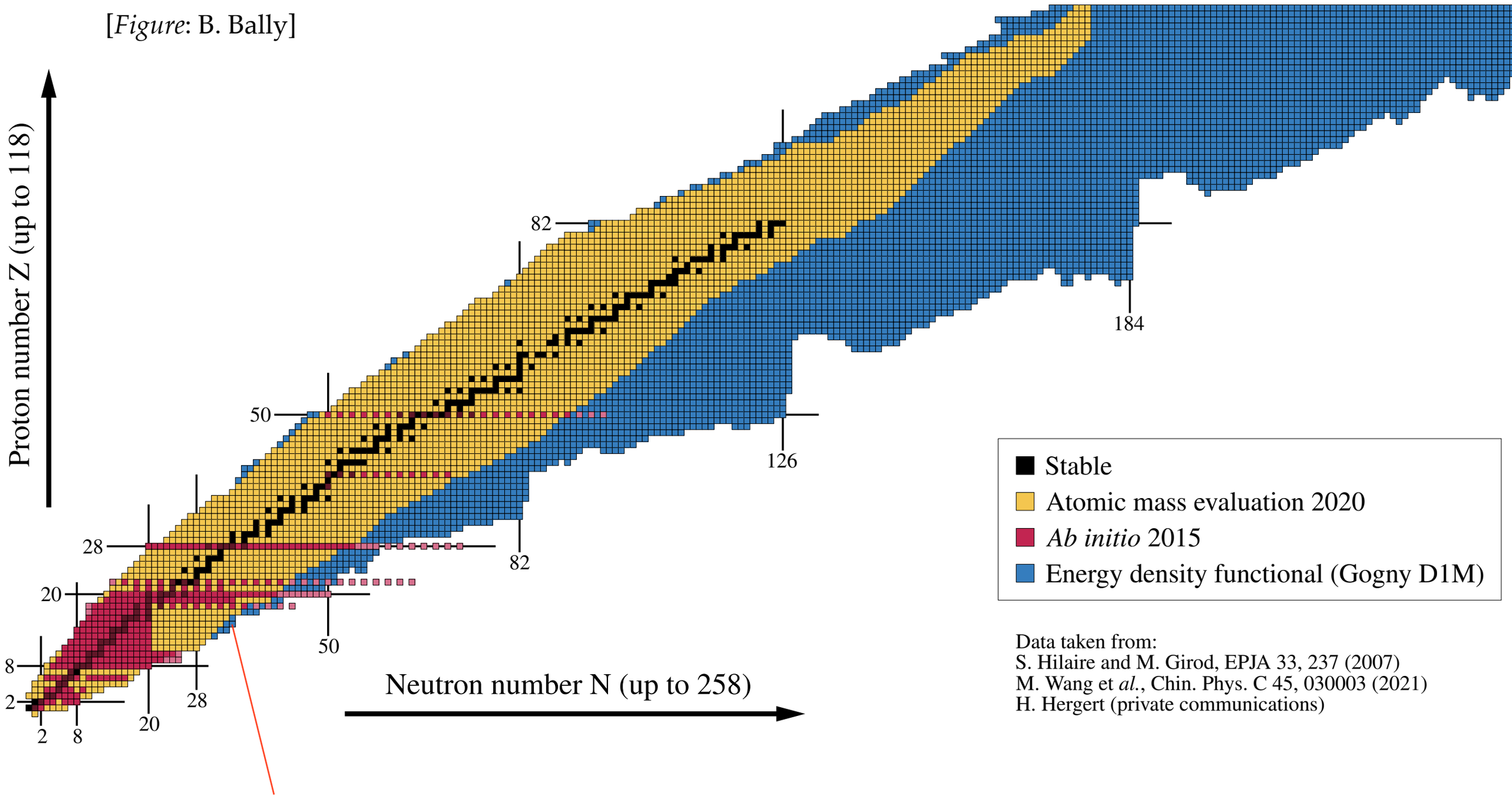


Data taken from:
S. Hilaire and M. Girod, EPJA 33, 237 (2007)
M. Wang et *al.*, Chin. Phys. C 45, 030003 (2021)
H. Hergert (private communications)

- Only exact methods available

Progress of ab initio calculations

[*Figure*: B. Bally]



Data taken from:
S. Hilaire and M. Girod, EPJA 33, 237 (2007)
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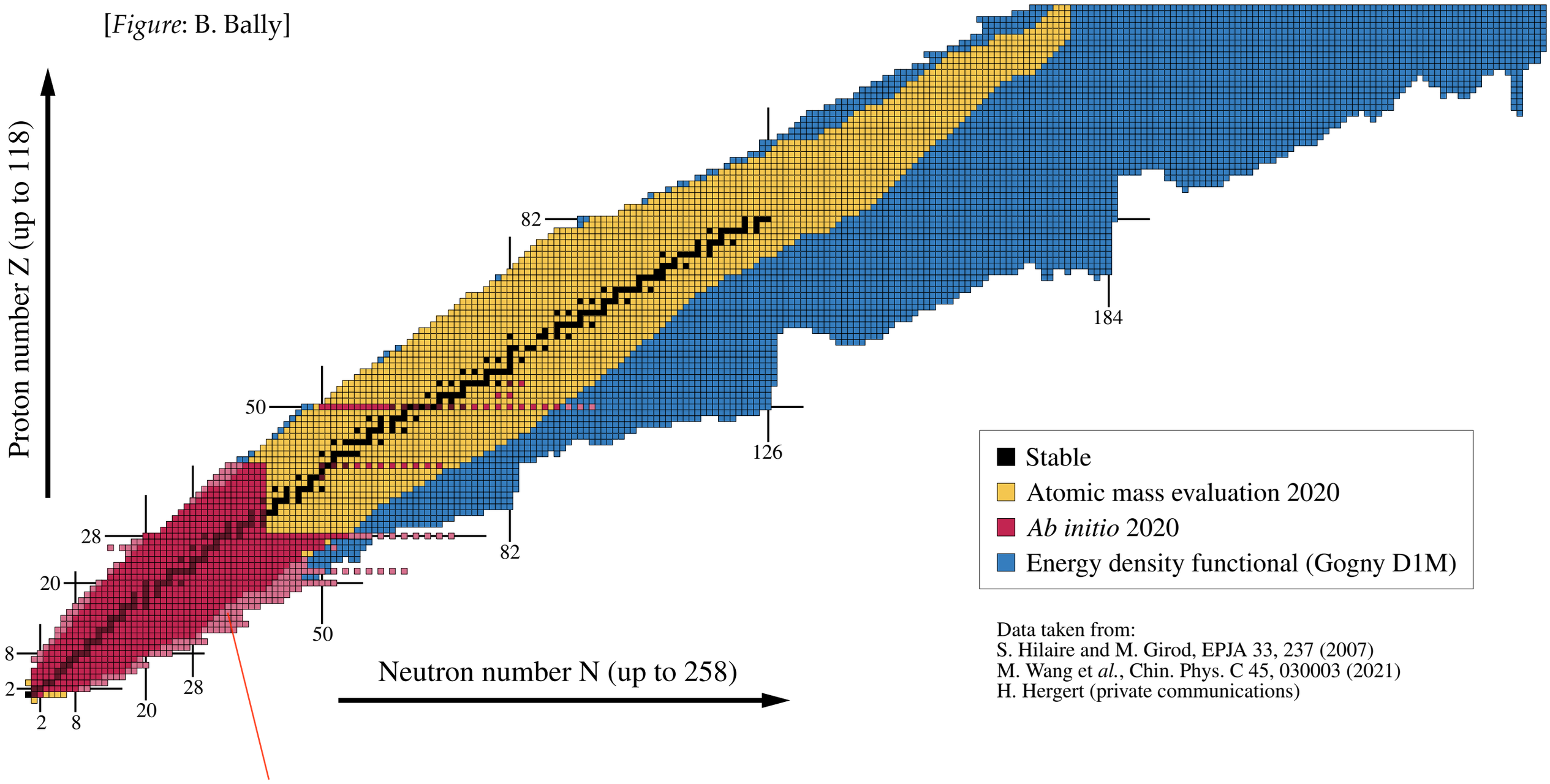
H. Hergert (private communications)

- Development of symmetry-conserving methods → **doubly closed-shell** nuclei
- Development of U(1) symmetry-breaking methods → **singly open-shell** nuclei

Progress of ab initio calculations

[*Figure*: B. Bally]



Data taken from:
S. Hilaire and M. Girod, EPJA 33, 237 (2007)
M. Wang et *al.*, Chin. Phys. C 45, 030003 (2021)
H. Hergert (private communications)

- Development of SU(2) symmetry-breaking methods → **doubly open-shell** nuclei

Open problems

- **Towards heavy nuclei**
  - Size of 3N matrix elements becomes prohibitive

  → Techniques from applied maths → Tensor factorisation of the many-body problem

- **Doubly open-shell nuclei**
  - Symmetry breaking? Single- or multi-reference? Scaling?

  → Strategy has to be adapted to the obejective

- **Uncertainty quantification**
  - Thorough quantification to establish link to QCD & predictive power

  → Development of efficient many-body *emulators* → Towards statistical analyses of LEC fits

  → Issue of renormalisability?

- **How far can this approach be pushed?**
  - Not obvious that "chiral EFT in the A-body sector" works all the way up to superheavy nuclei

  → Different types of EFT explored

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