Ab Initio Valence-Space Hamiltonians and Operators from In-Medium SRG

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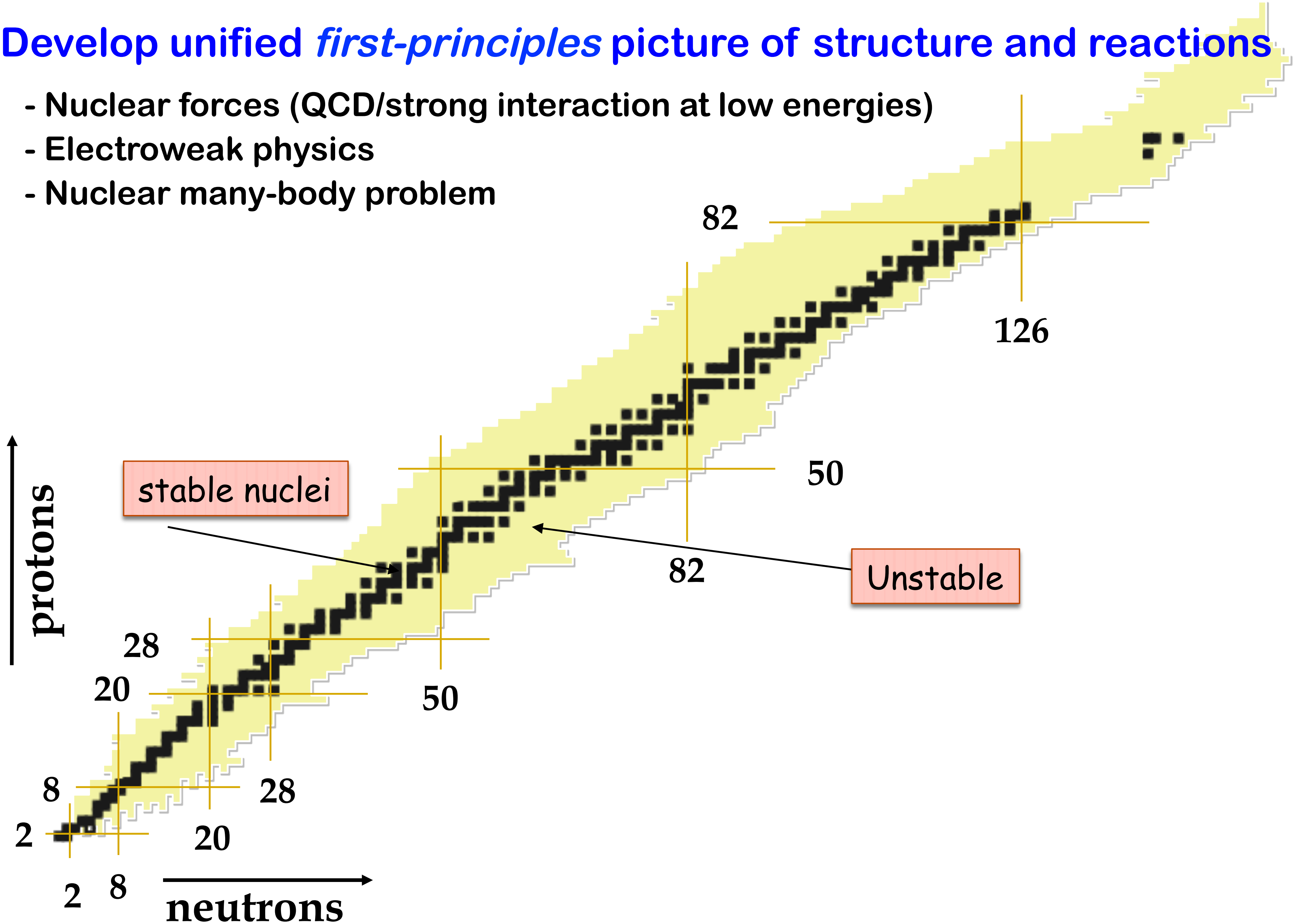
Frontiers and Impact of Nuclear Science

Aim of modern nuclear theory:

Develop unified *first-principles* picture of structure and reactions

- Nuclear forces (QCD/strong interaction at low energies)
- Electroweak physics
- Nuclear many-body problem



Advances in Ab Initio Nuclear Structure for Medium-Mass Exotic Nuclei

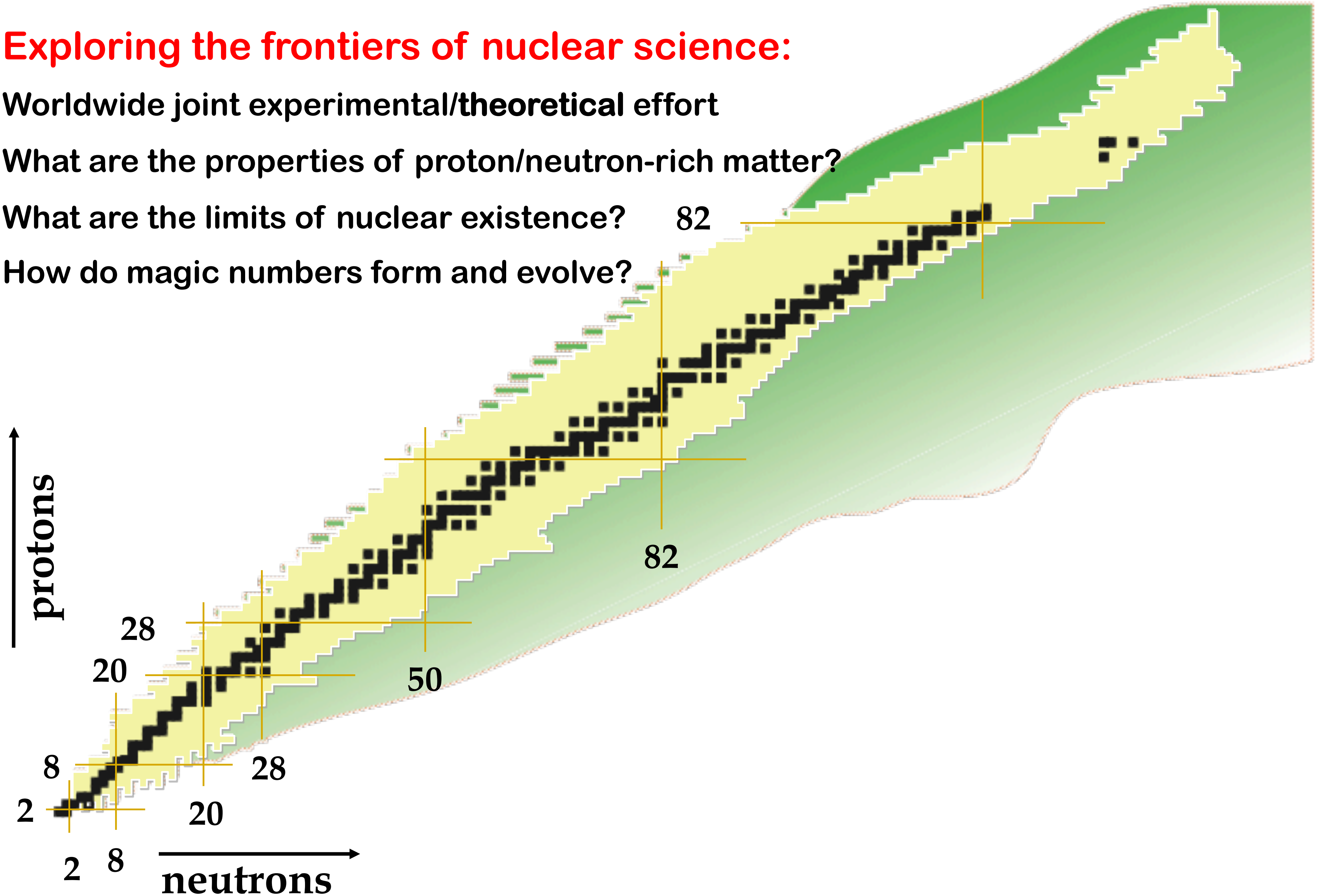
Exploring the frontiers of nuclear science:

Worldwide joint experimental/**theoretical** effort

What are the properties of proton/neutron-rich matter?

What are the limits of nuclear existence?

How do magic numbers form and evolve?



Medium- and Heavy-Mass Exotic Nuclei

What are the properties of proton/neutron-rich matter?

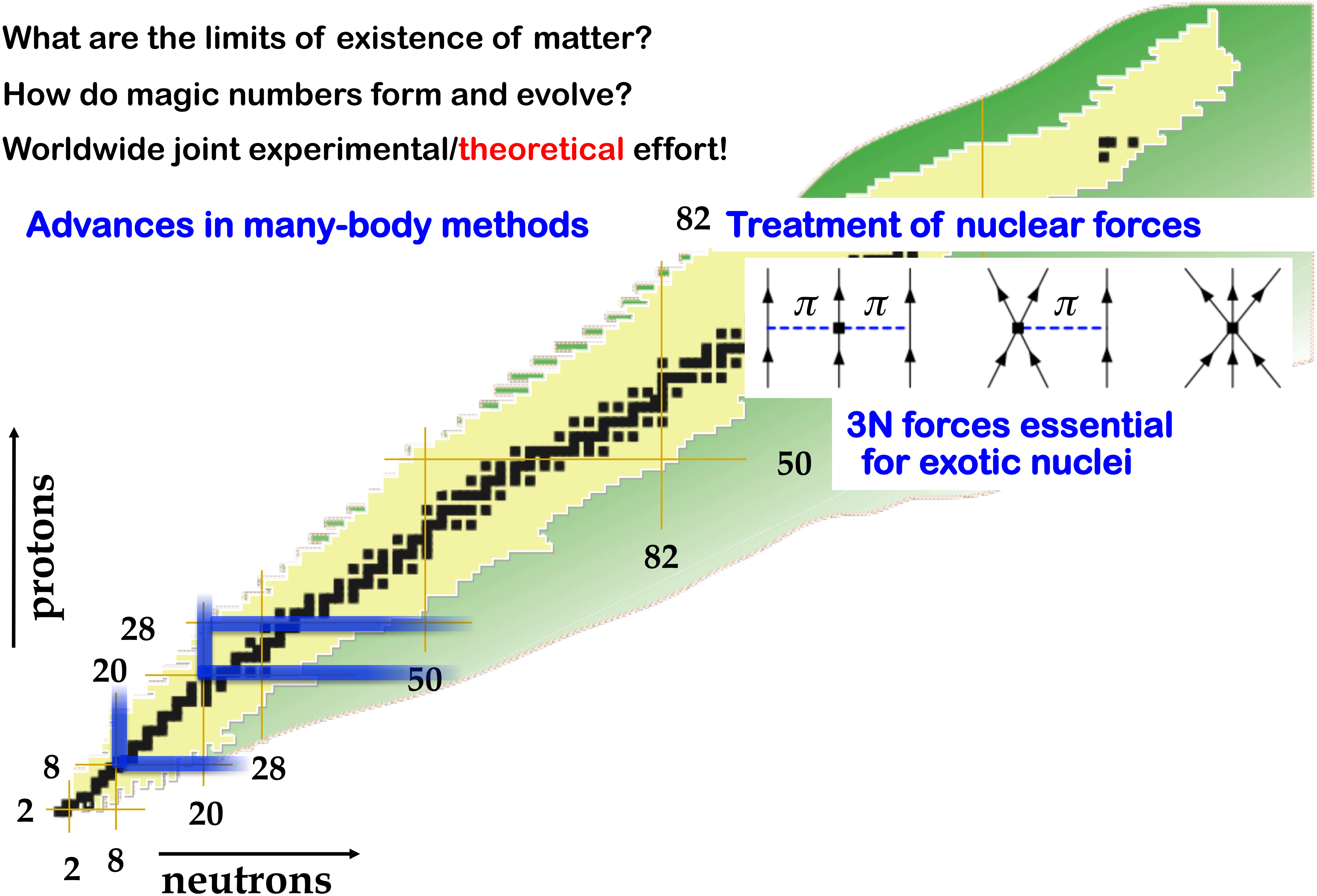
What are the limits of existence of matter?

How do magic numbers form and evolve?

Worldwide joint experimental/theoretical effort!

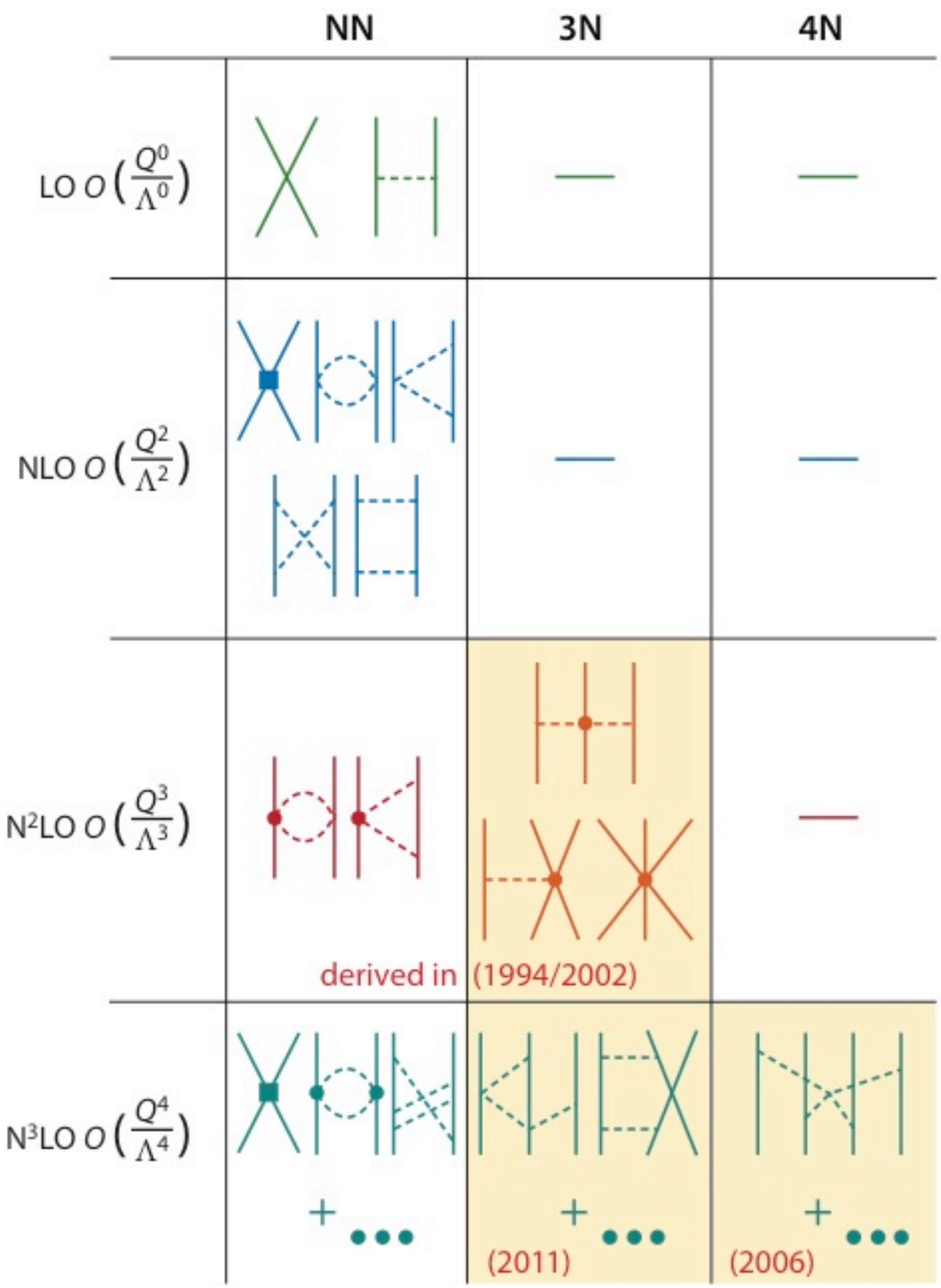
Advances in many-body methods

Treatment of nuclear forces



3N forces essential for exotic nuclei

Chiral Effective Field Theory: Nuclear Forces



Weinberg, van Kolck, Kaplan, Savage, Wise

Nucleons interact via pion exchanges and contact interactions

Consistent treatment of NN, 3N,…

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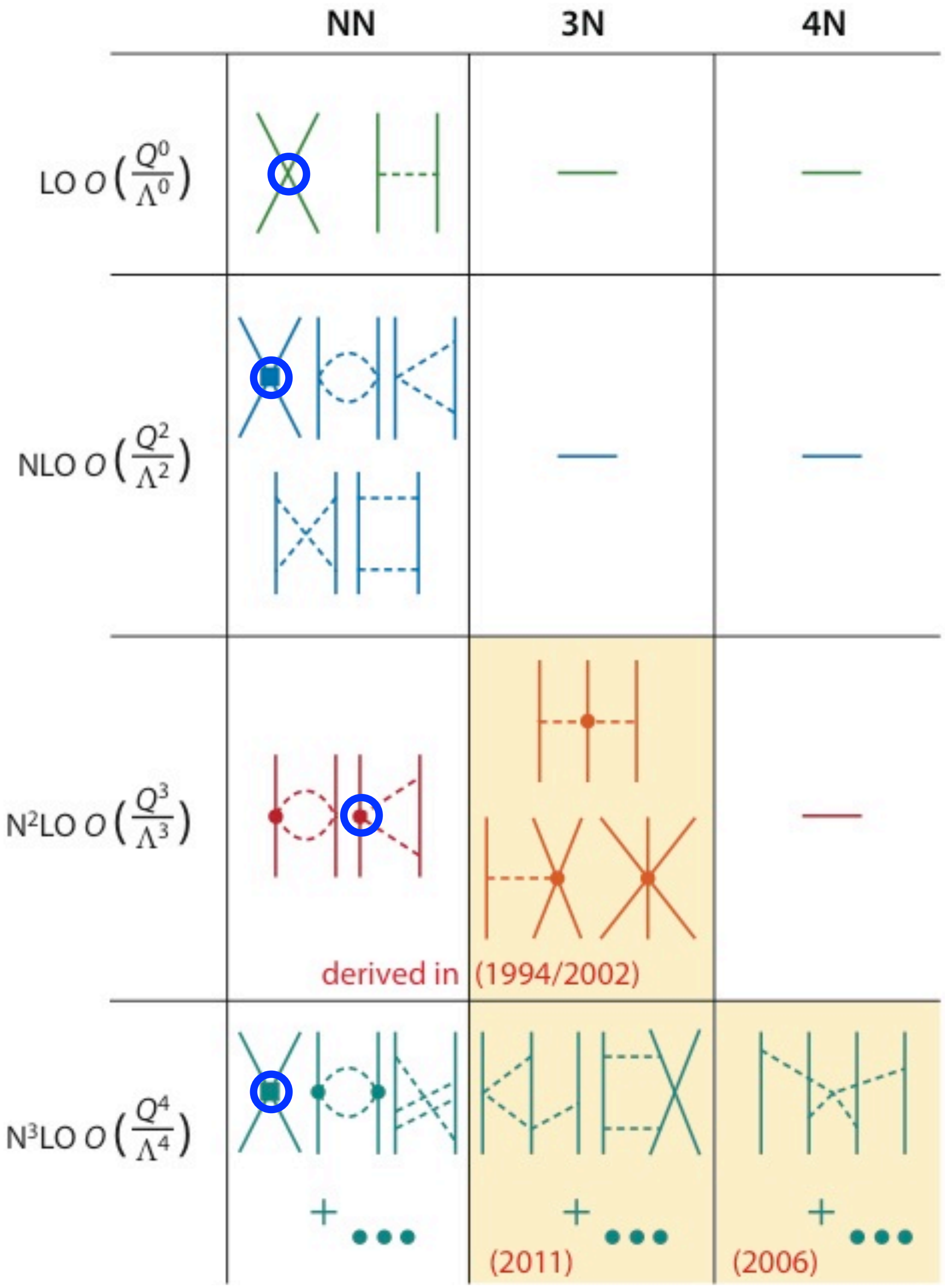

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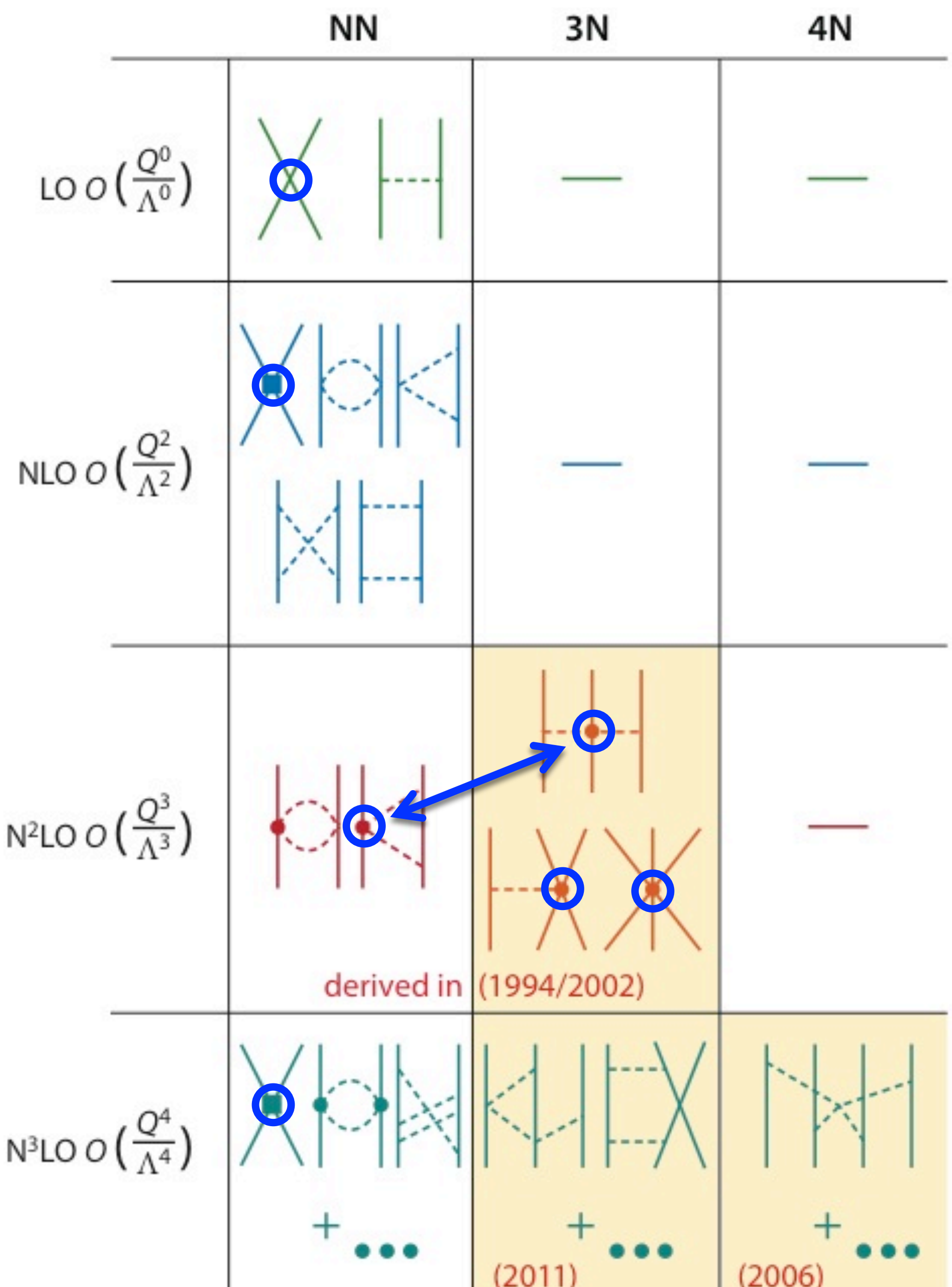

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3N couplings fit to 3/4-body systems

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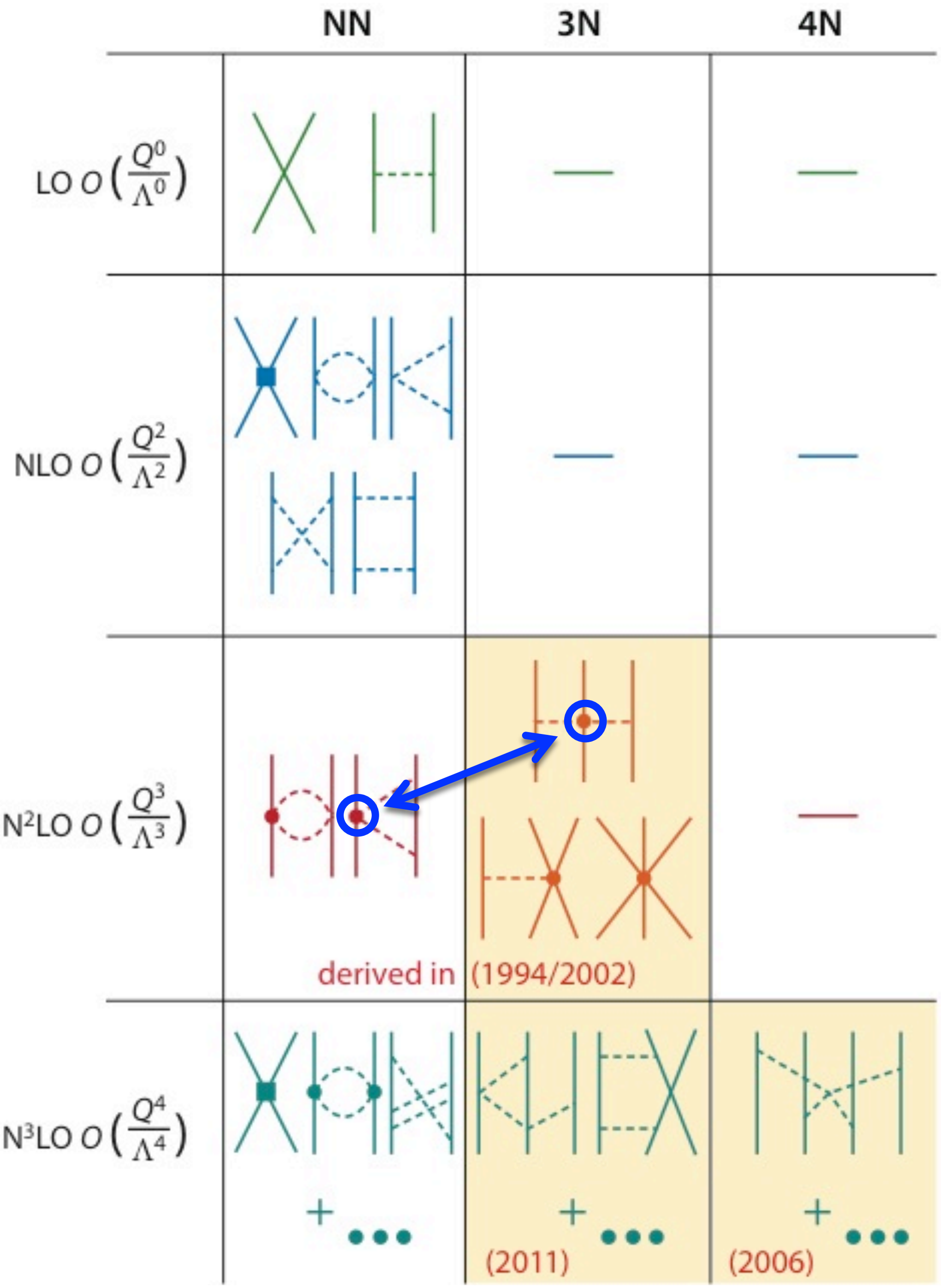


Weinberg, van Kolck, Kaplan, Savage, Wise…

Nucleons interact via pion exchanges and contact interactions

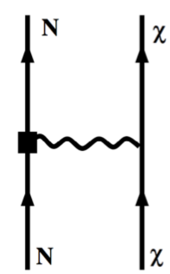
Consistent treatment of NN, 3N,…

NN couplings fit to scattering data

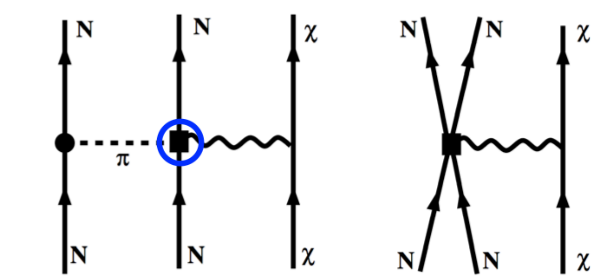
3N couplings fit to 3/4-body systems

Consistent EW/WIMP interactions

one-body currents at Q^0 and Q^2



+ two-body currents at Q^3



The Nuclear Many-Body Problem

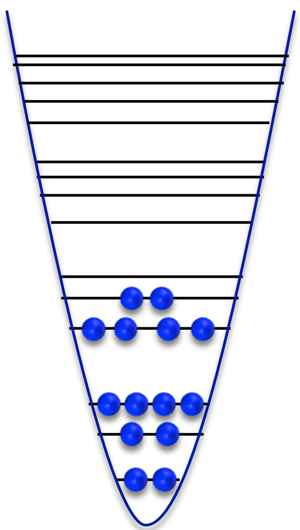
Nucleus strongly interacting many-body system – how to solve A-body problem?

$$H\psi_n = E_n\psi_n$$

Quasi-exact solutions only in light nuclei (GFMC, NCSM, …)

Large scale: controlled approximations to full Schrödinger Equation

Large-scale approaches



Limited range:

Closed shell ± 1

Even-even

Limited properties:

Ground states only

Some excited state

Coupled Cluster

In-Medium SRG

Green's Function

Unitary model operator

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Nucleus strongly interacting many-body system – how to solve A-body problem?

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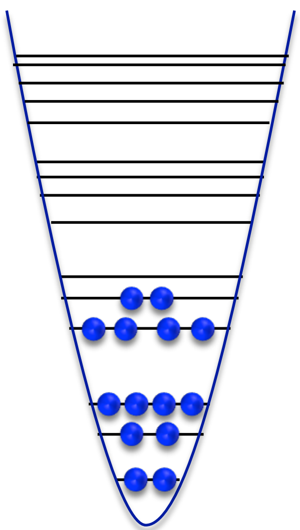
Large scale: controlled approximations to full Schrödinger Equation

Valence space: diagonalize exactly with reduced number of degrees of freedom

Large-scale approaches



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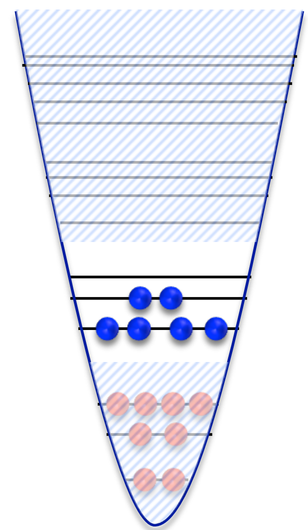


All nuclei near

closed-shell cores

All properties:

Ground states

Excited states

EW transitions

Coupled Cluster

In-Medium SRG

Perturbation Theory

Valence-Space Philosophy

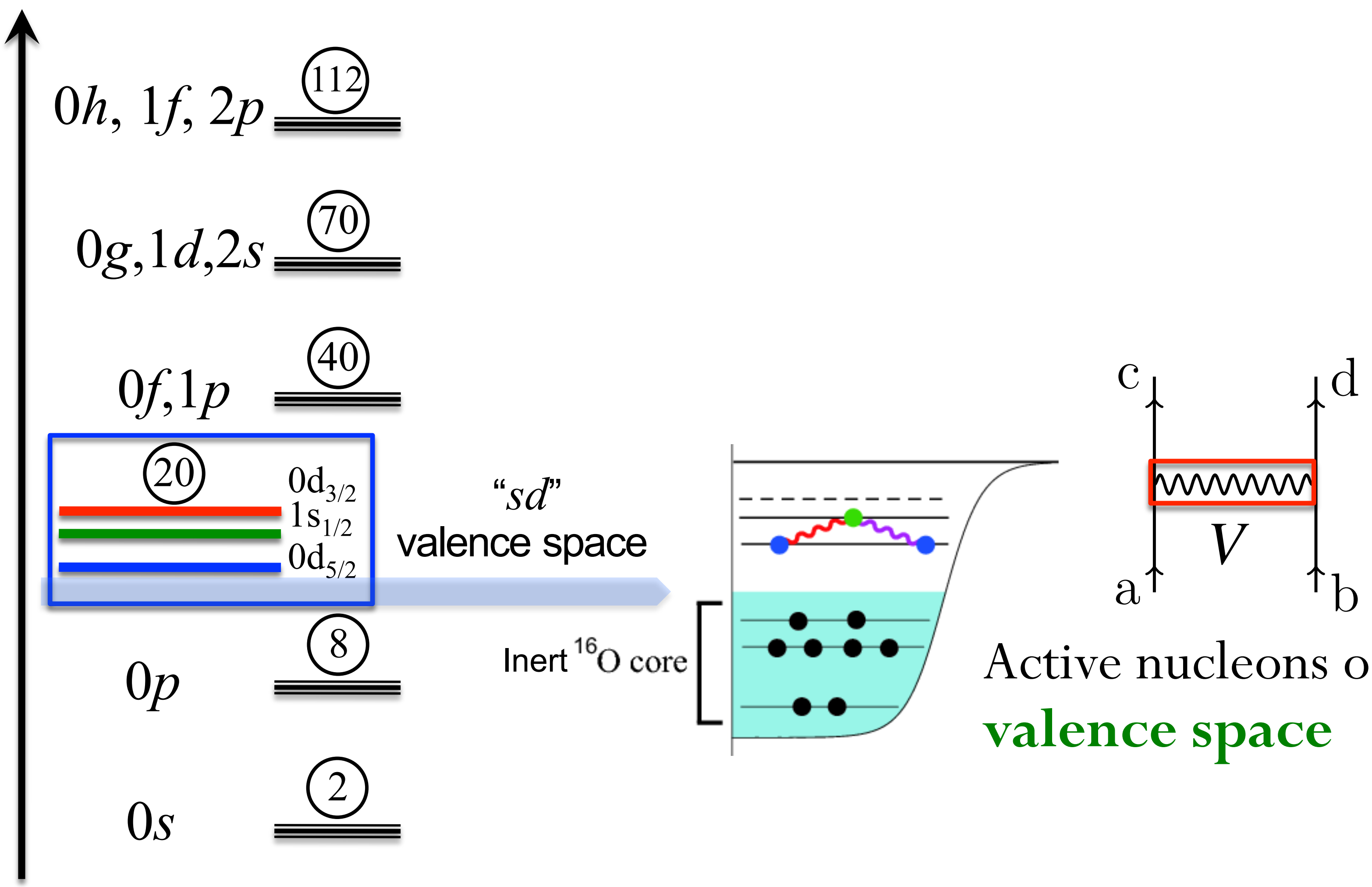
Nuclei understood as many-body system starting from closed shell, add nucleons

Valence-space Hamiltonian derived from nuclear forces:

Single-particle energies

Interaction matrix elements

$$H_{\text{v.s.}} = \sum_i \varepsilon_i a_i^\dagger a_i + V_{\text{v.s.}}$$



Active nucleons occupy **valence space**

Valence-Space Philosophy

Nuclei understood as many-body system starting from closed shell, add nucleons

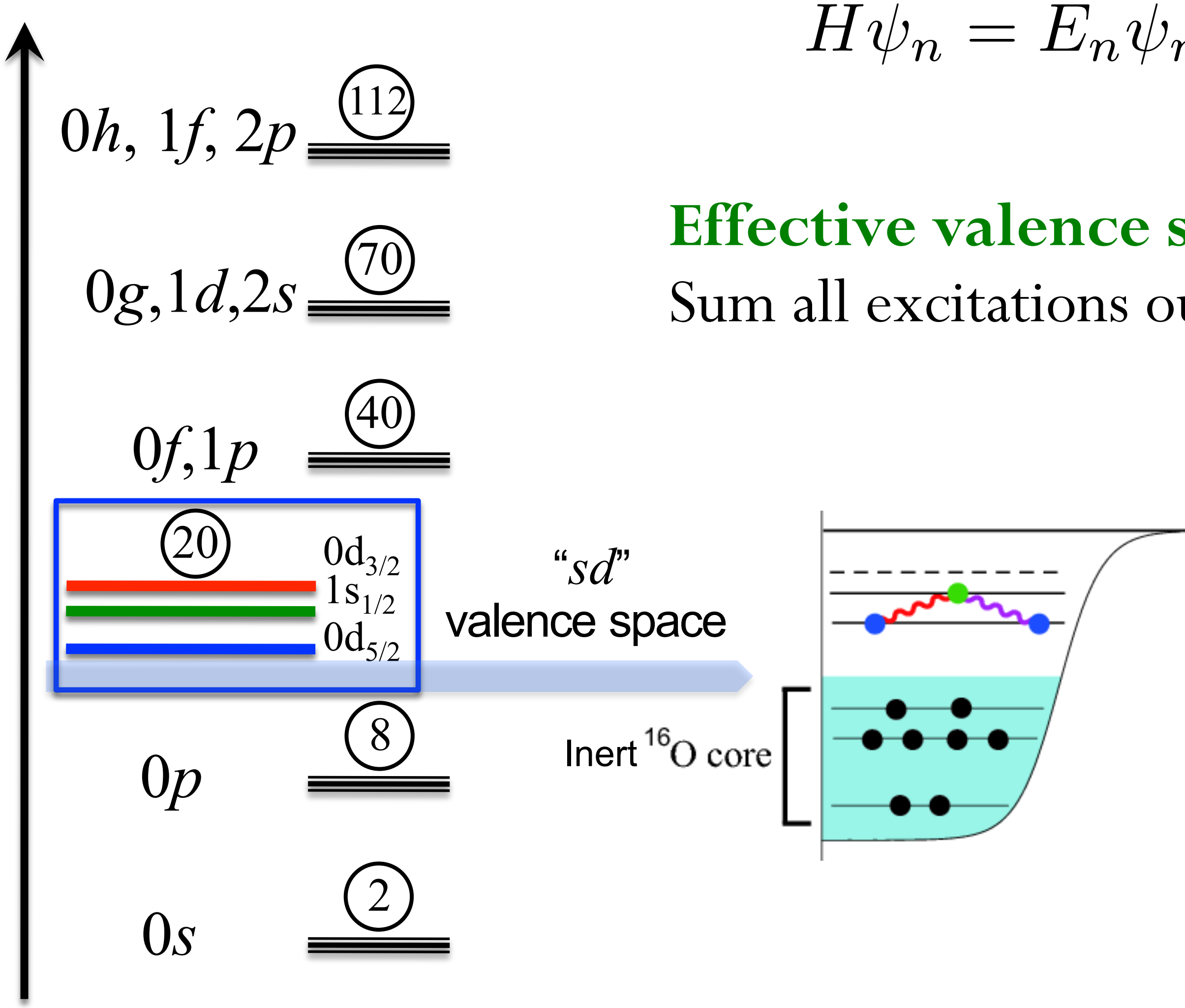
Valence-space Hamiltonian derived from nuclear forces:

Single-particle energies

Interaction matrix elements

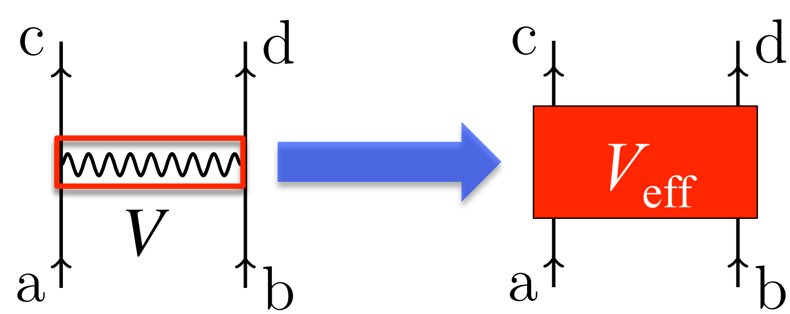
$$H_{\text{eff}} = \sum_i \varepsilon_{i_{\text{eff}}} a_i^\dagger a_i + V_{\text{eff}}$$

$$H\psi_n = E_n\psi_n \rightarrow PH_{\text{eff}}P\psi_i = E_iP\psi_i$$



Effective valence space Hamiltonian:

Sum all excitations outside valence space



Decouple valence space from excitations

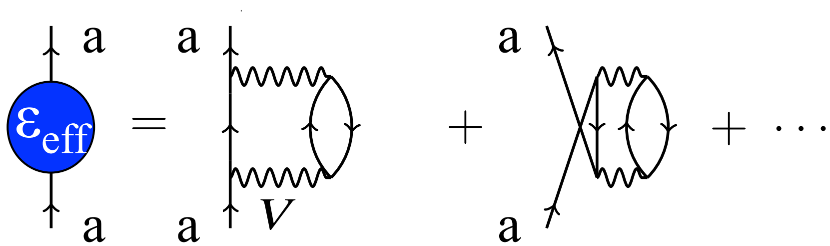
Perturbative Approach

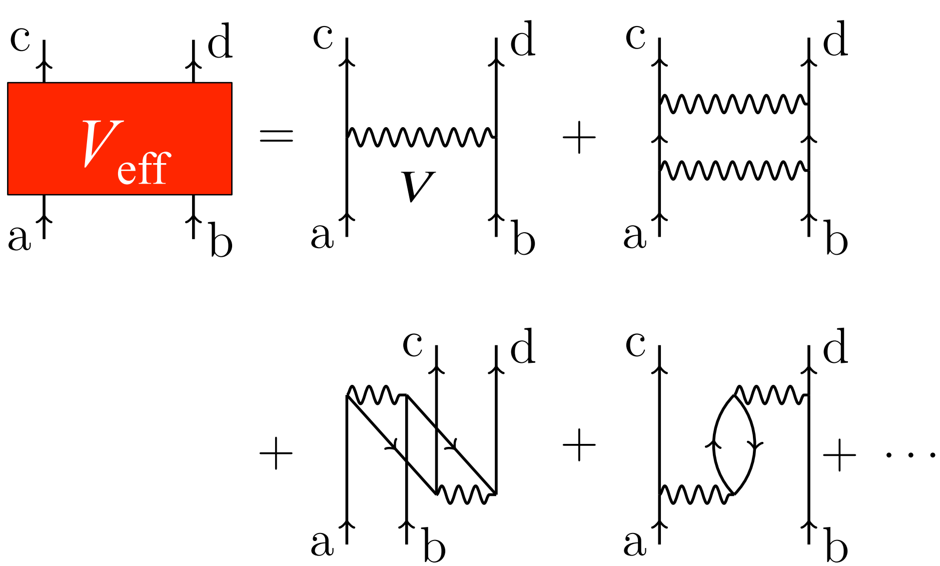
1) Effective Hamiltonian: sum excitations outside valence space to **MBPT(3)**

2) Self-consistent single-particle energies

3) **Harmonic-oscillator** basis of 13-15 major shells: **converged**

4) NN and 3N forces from chiral EFT





Perturbative Approach

1) Effective Hamiltonian: sum excitations outside valence space to MBPT(3)
2) Self-consistent single-particle energies
3) Harmonic-oscillator basis of 13-15 major shells
4) NN and 3N forces from chiral EFT

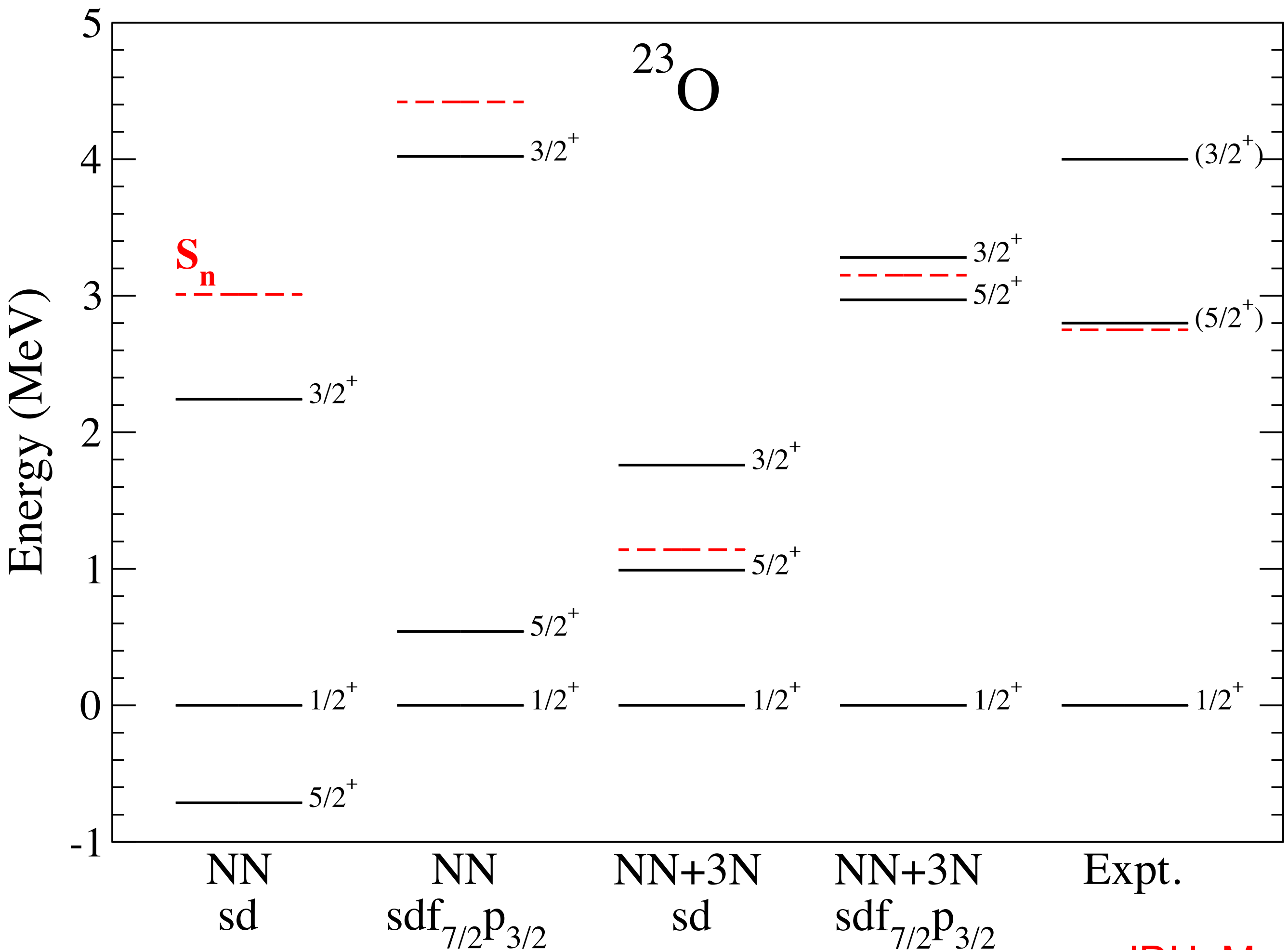
<u>Undesirable Features</u>

- Uncertain perturbative convergence
- Core physics inconsistent or absent
- Degenerate valence space requires HO basis (HF requires nontrivial extension)
- Must treat additional orbitals nonperturbatively (extend valence space)

Impact on Spectra: ^{23}O

Neutron-rich oxygen spectra with NN+3N

$5/2^+$, $3/2^+$ energies reflect ^{22,24}O shell closures



***sd*-shell NN only**

Wrong ground state

$5/2^+$ too low

$3/2^+$ bound

NN+3N

Clear improvement in extended valence space

JDH, Menéndez, Schwenk, EPJA (2013)

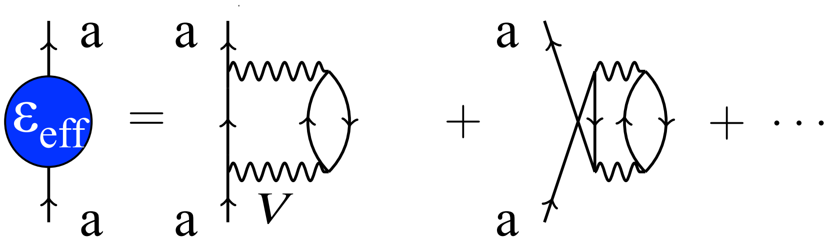
Perturbative Approach

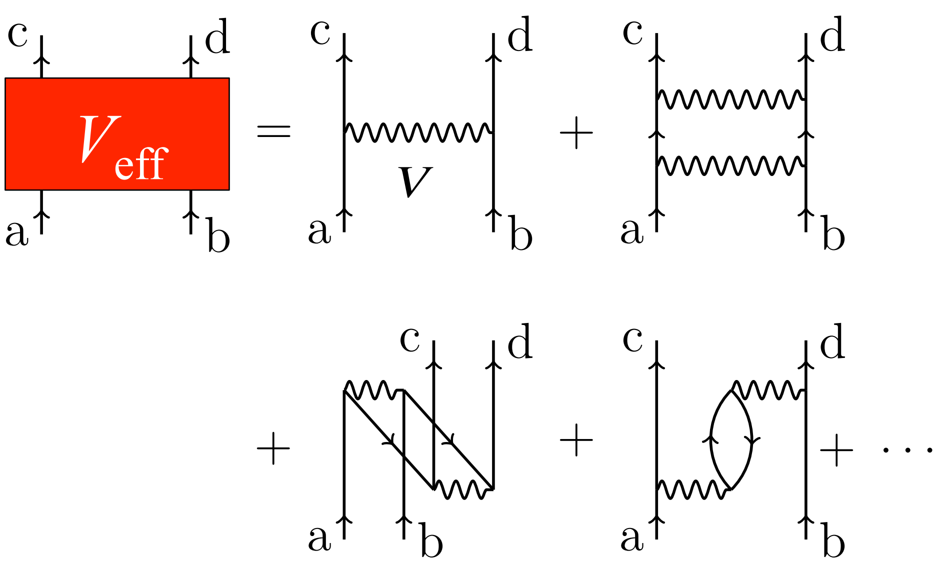
1) Effective Hamiltonian: sum excitations outside valence space to MBPT(3)

2) Self-consistent single-particle energies

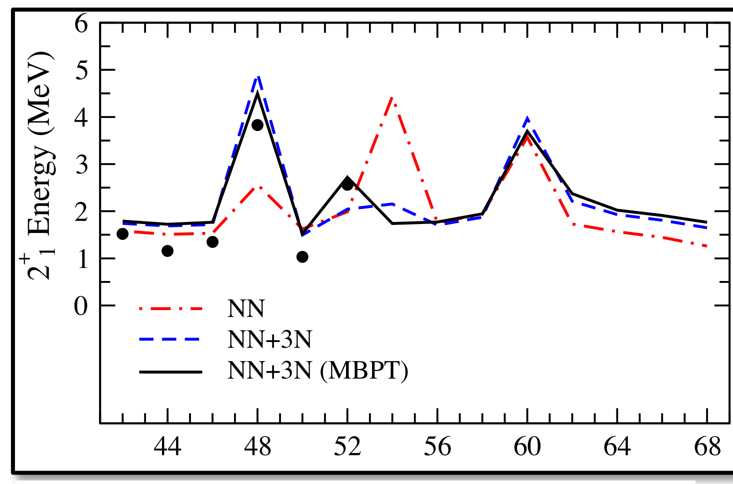
3) Harmonic-oscillator basis of 13–15 major shells

4) NN and **3N forces** from chiral EFT – to 3rd-order MBPT

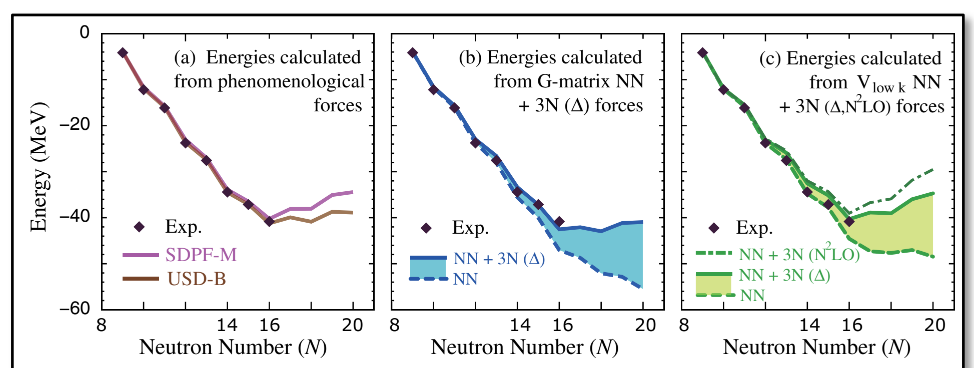




New magic numbers in calcium



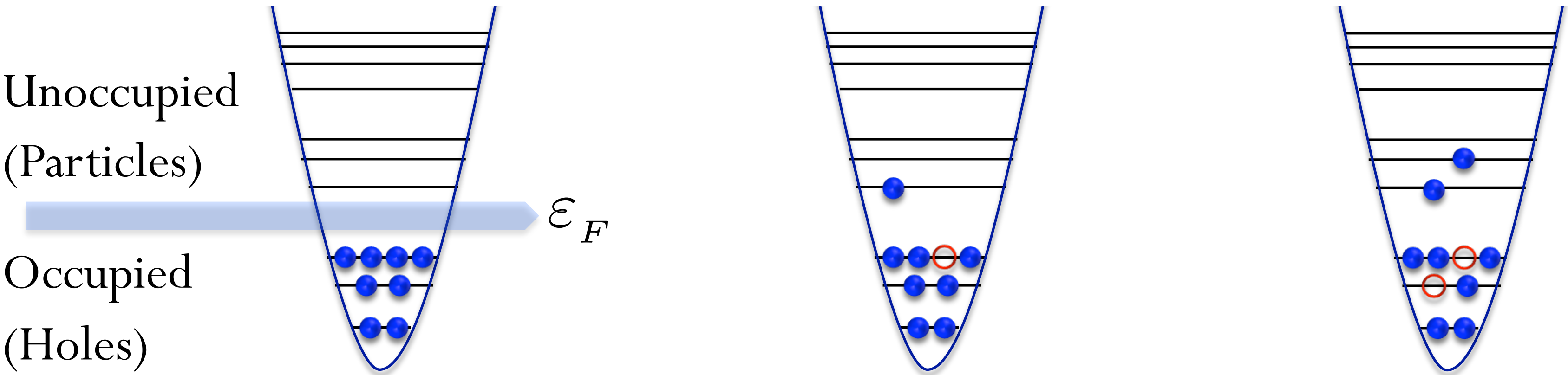
Heaviest oxygen isotope



Particle/Hole Excitations

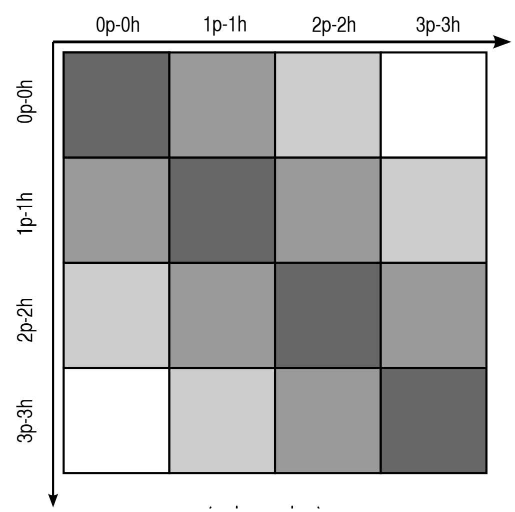
Consider basis states as excitations from some reference state:

Reference Slater Determinant | 1p-1h excitation | 2p-2h excitation



$$|\Phi\rangle = \prod_{i=1}^{N} a_i^\dagger |0\rangle \qquad |\Phi_i^a\rangle = a_a^\dagger a_i |\Phi\rangle \qquad |\Phi_{ij}^{ab}\rangle = a_a^\dagger a_i a_b^\dagger a_j |\Phi\rangle$$

Hamiltonian schematically given in terms of ph excitations



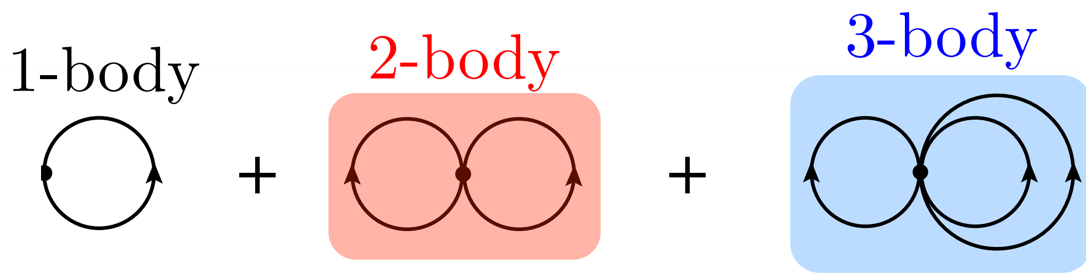
$\langle i|H|j\rangle$

Normal-Ordered Hamiltonian

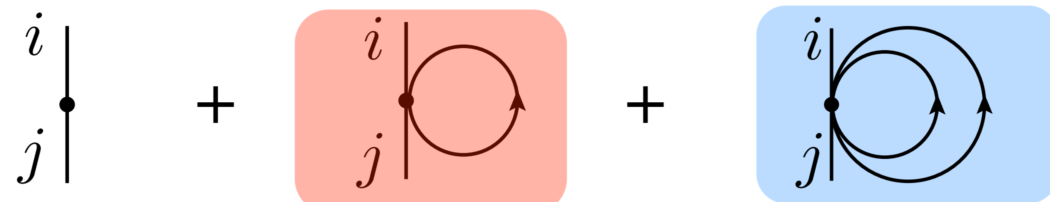
Now rewrite exactly the initial Hamiltonian in normal-ordered form

$$H_{\text{N.O.}} = E_0 + \sum_{ij} f_{ij} \left\{a_i^\dagger a_j\right\} + \frac{1}{4}\sum_{jkl} \Gamma_{ijkl} \left\{a_i^\dagger a_j^\dagger a_l a_k\right\} + \frac{1}{36}\sum_{ijklmn} W_{ijklmn} \left\{a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n\right\}$$

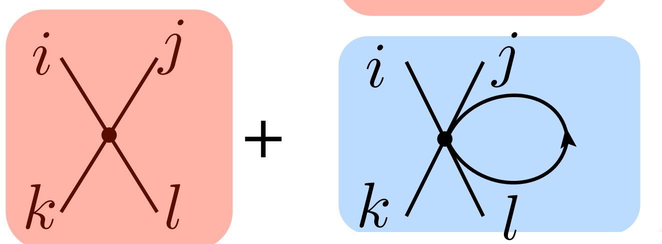
$$\text{N.O. 0-body} \rightarrow E_0 =$$



$$\text{N.O. 1-body} \rightarrow \quad f =$$



$$\text{N.O. 2-body} \rightarrow \quad \Gamma =$$



Normal-ordered Hamiltonian w.r.t. reference state

Loop = **sum over occupied states**

Include dominant 1-,2-,3-body physics in NO

Nonperturbative In-Medium SRG

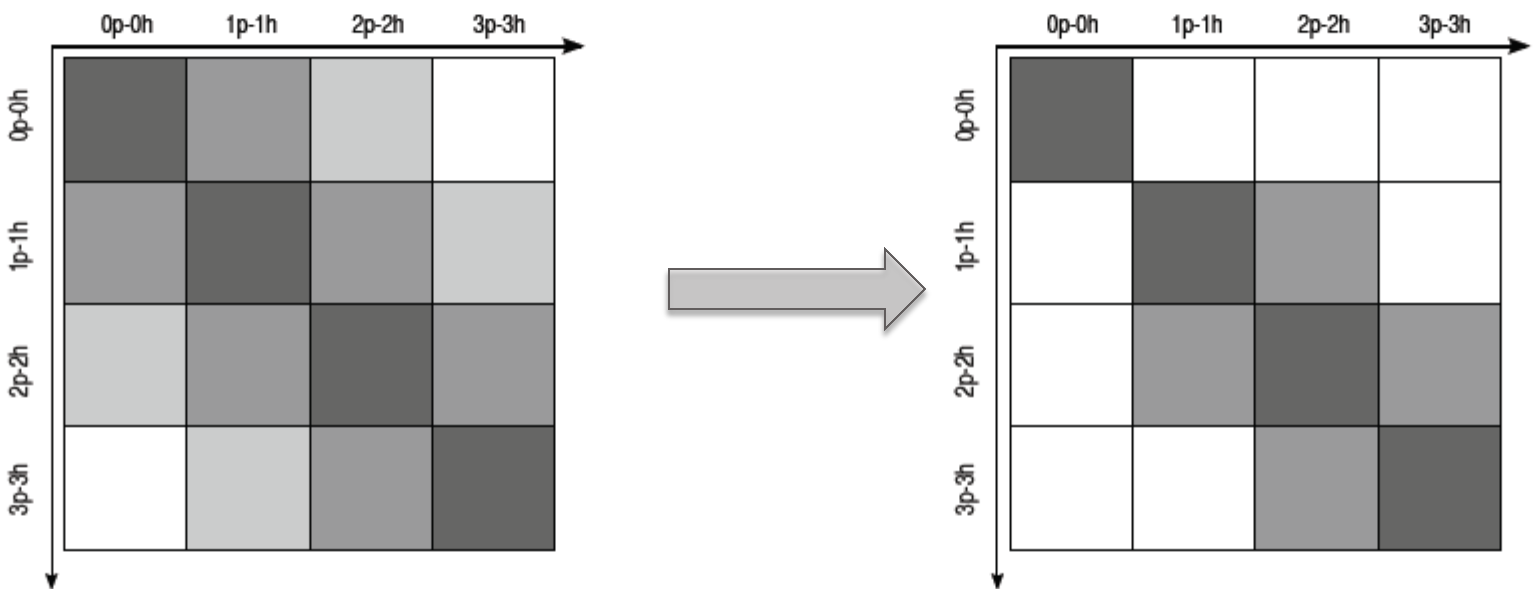
Tsukiyama, **Bogner**, Schwenk, PRL (2011)

In-Medium SRG continuous unitary trans. drives off-diagonal physics to zero

$$H(s) = U(s) H U^\dagger(s) \equiv H^{\mathrm{d}}(s) + H^{\mathrm{od}}(s) \to H^{\mathrm{d}}(\infty)$$

From uncorrelated Hartree-Fock ground state (e.g., ^{16}O) define:

$$H^{\mathrm{od}} = \langle p|H|h\rangle + \langle pp|H|hh\rangle + \cdots + \text{h.c.}$$



$\langle i|H|j\rangle$ $\qquad$ $\langle \mathrm{np}\mathrm{n}h|H(\infty)|\Phi_{\mathrm{core}}\rangle = 0$

Drives all n-particle n-hole couplings to 0 – decouples core from excitations

IM-SRG: Flow Equation Formulation

Define *U(s)* implicitly from particular choice of generator:

$$\eta(s) \equiv (\mathrm{d}U(s)/\mathrm{d}s)\, U^\dagger(s)$$

chosen for desired decoupling behavior – e.g.,

$$\eta_I(s) = \left[H^{\mathrm{d}}(s), H^{\mathrm{od}}(s)\right]$$ Wegner (1994)

Solve **flow equation** for Hamiltonian (coupled DEs for 0,1,2-body parts)

$$\frac{\mathrm{d}H(s)}{\mathrm{d}s} = [\eta(s), H(s)] \qquad H(s) = E_0(s) + f(s) + \Gamma(s) + \cdots$$

Hamiltonian and generator truncated at 2-body level: **IM-SRG(2)**

0-body flow drives uncorrelated ref. state to fully correlated ground state

$$E_0(\infty) \to \text{Core Energy}$$

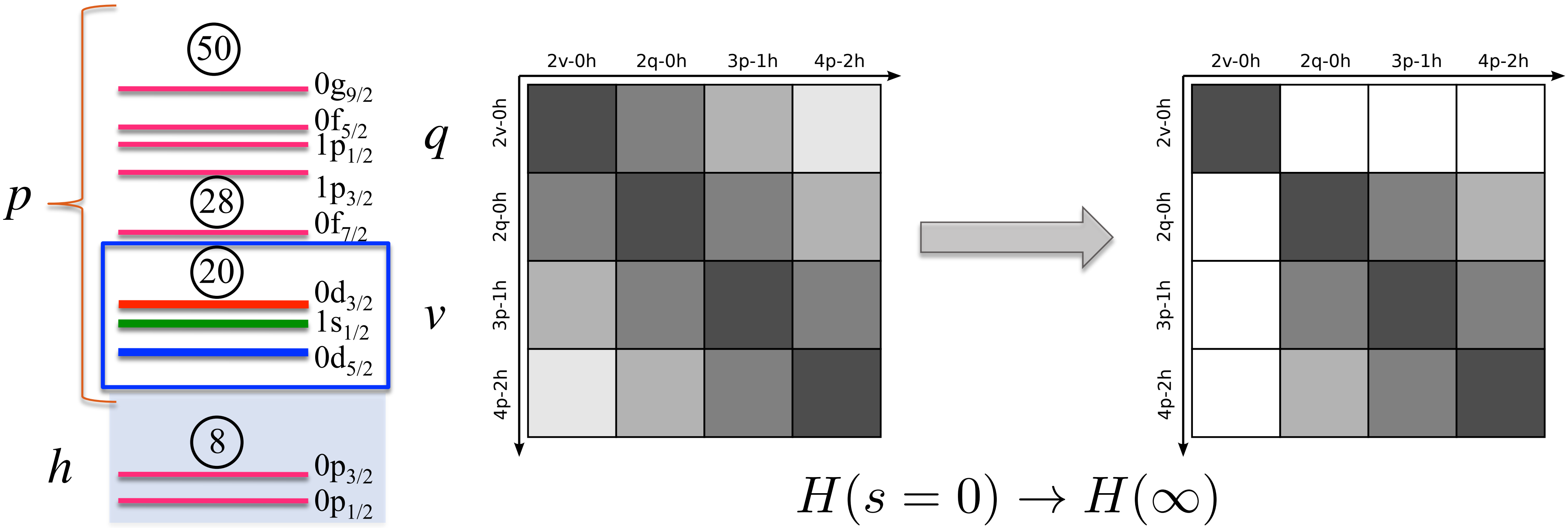
Ab initio method for energies of **closed-shell systems**

IM-SRG: Valence-Space Hamiltonians

Tsukiyama, **Bogner**, Schwenk, PRC (2012)

Open-shell systems

Separate p states into valence states (v) and those above valence space (q)



$$H(s=0) \to H(\infty)$$

Redefine H^{od} to **decouple valence space from excitations** outside v

$$H^{\text{od}} = \langle p|H|h\rangle + \langle pp|H|hh\rangle + \langle v|H|q\rangle + \langle pq|H|vv\rangle + \langle pp|H|hv\rangle + \text{h.c.}$$

$E_0(\infty) \to \text{Core Energy}$ $\quad f(\infty) \to \text{SPEs}$ $\quad \Gamma(\infty) \to V_{\text{eff}}$

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Tsukiyama, **Bogner**, Schwenk, PRC (2012)

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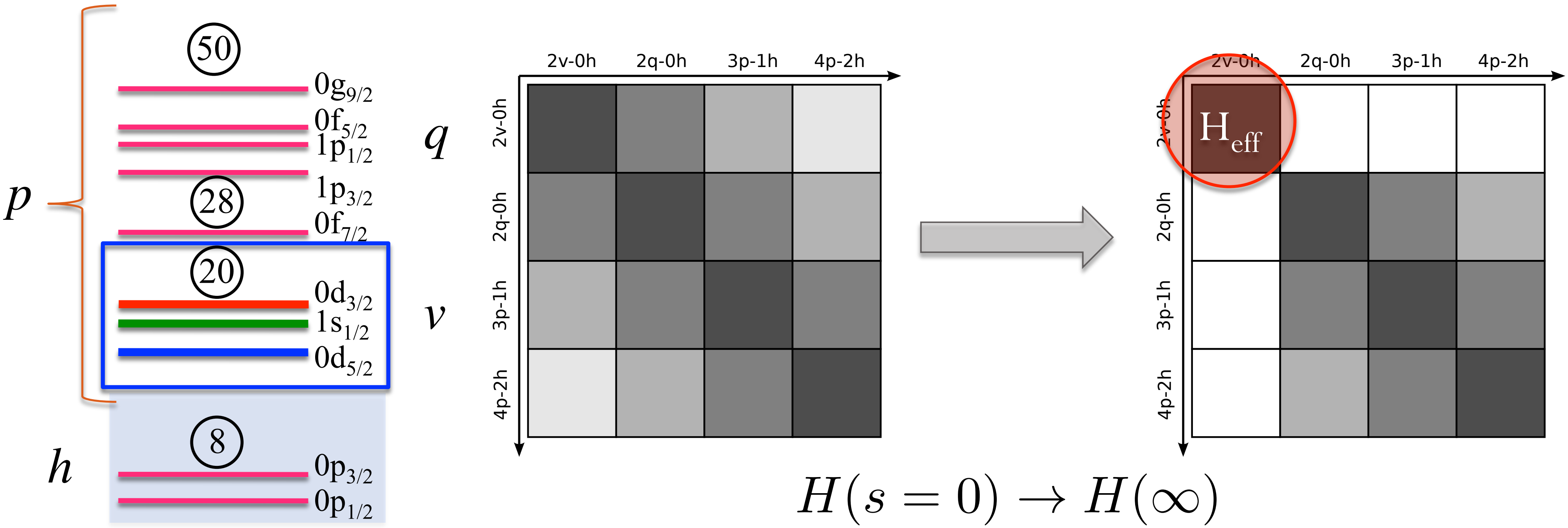
Separate *p* states into valence states (*v*) and those above valence space (*q*)



$$H(s=0) \to H(\infty)$$

Core physics included consistently (**absolute energies, radii…**)

Inherently nonperturbative – no need for extended valence space

Non-degenerate valence-space orbitals

Nonperturbative Valence-Space Strategy

1) NN and 3N forces from Chiral EFT
2) Evolve with free-space SRG
3) Normal-order w.r.t. HF reference state
4) Perform IM-SRG(2) calculation in flow-equation approach
5) Diagonalize with standard shell-model machinery

NN matrix elements

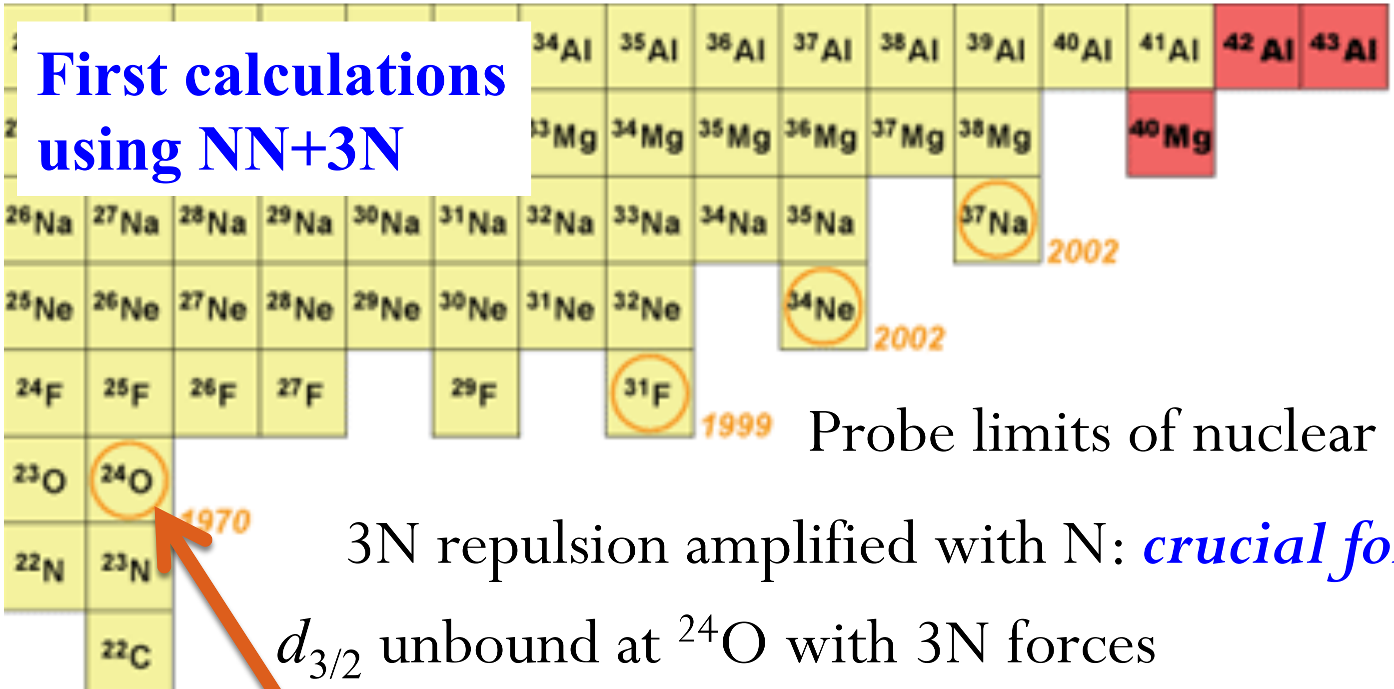
- $e_{\max} = 2n + l = 14$ **converged**
- Vary $\hbar\omega = 20 - 24\,\mathrm{MeV}$
- Consistently include 3N forces **induced** by SRG evolution (**NN+3N-ind**)

Initial 3N force contributions

- Chiral N^2LO (**NN+3N-full**)
- Included with cut: $e_1 + e_2 + e_3 \leq E_{3\max} = 14$

Oxygen Anomaly

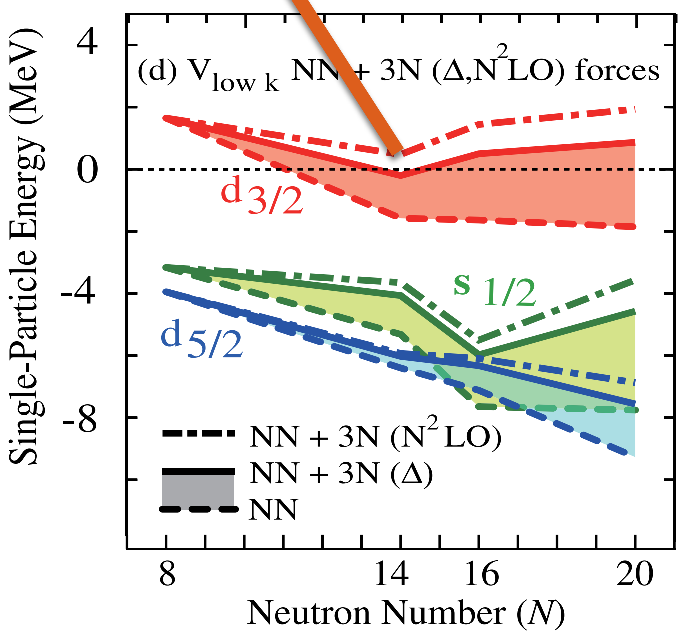
First calculations using NN+3N

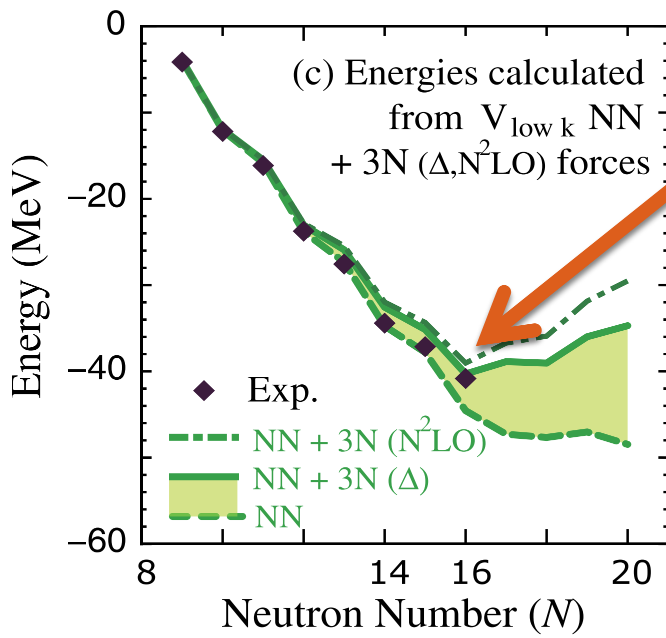


Probe limits of nuclear existence with 3N forces

3N repulsion amplified with N: ***crucial for neutron-rich nuclei***

$d_{3/2}$ unbound at ^{24}O with 3N forces





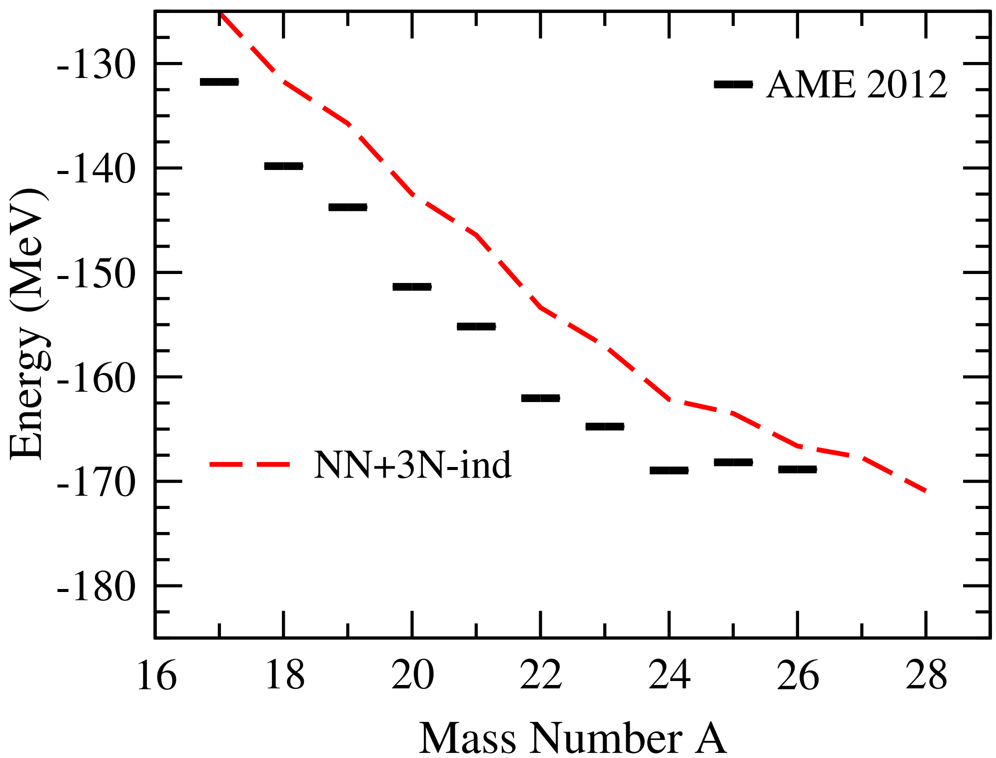
Isotopes unbound beyond ^{24}O

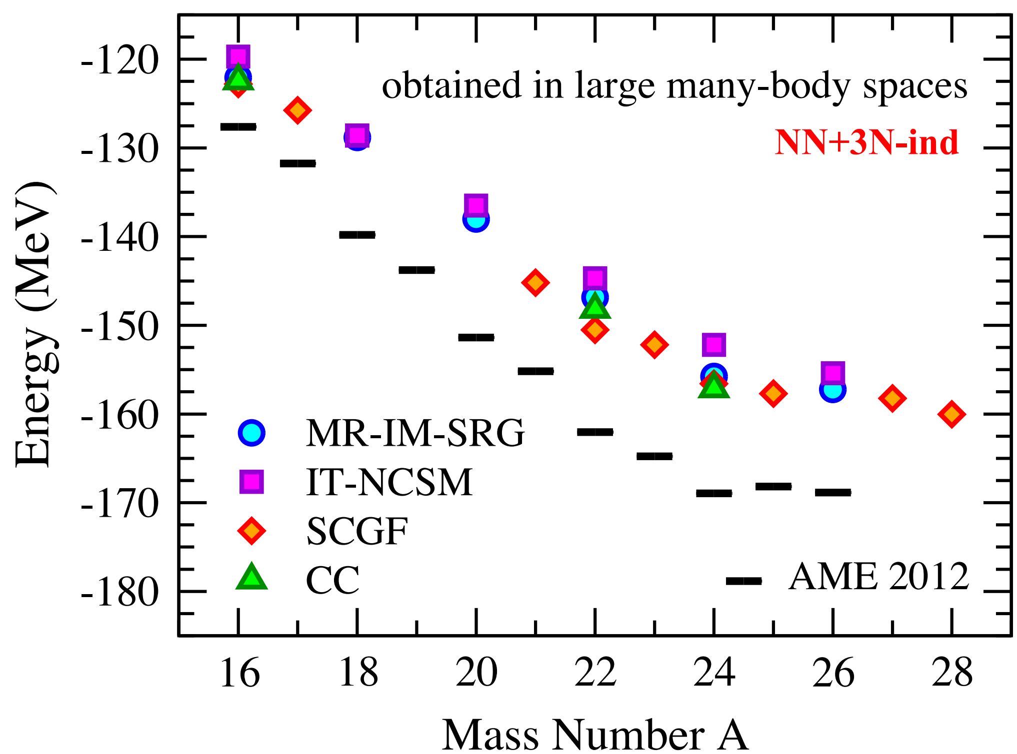
First microscopic explanation of oxygen anomaly

Otsuka, Suzuki, JDH, Schwenk, Akaishi, PRL (2010)

Comparison with Large-Space Methods

Large-space methods with **same SRG-evolved NN+3N-ind forces**



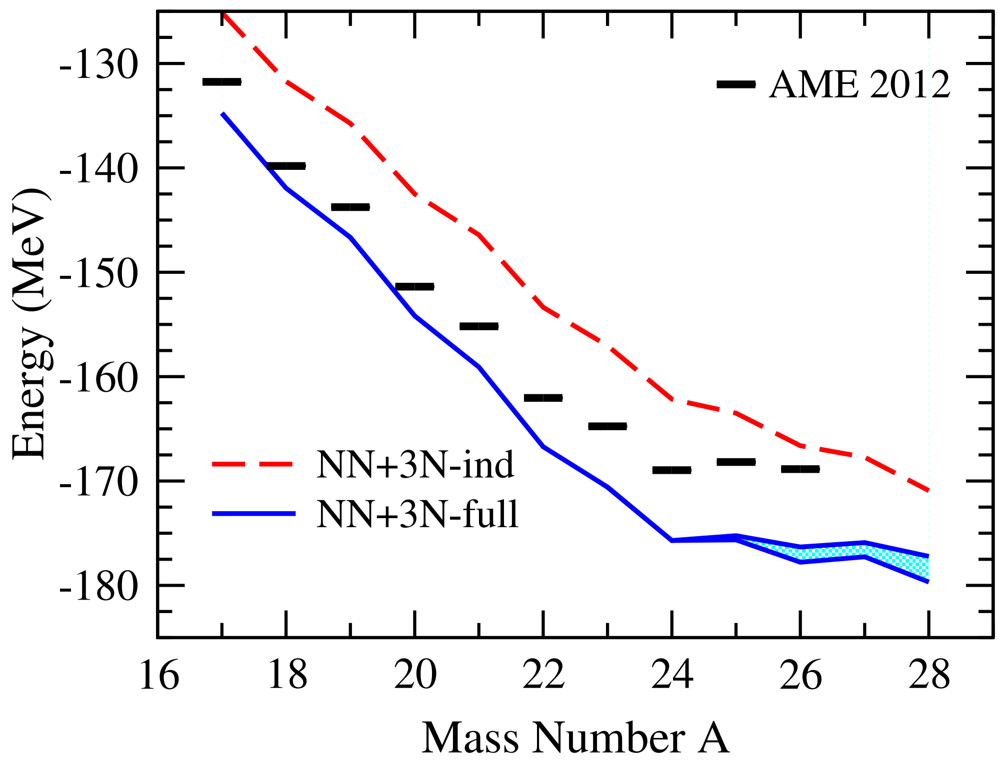


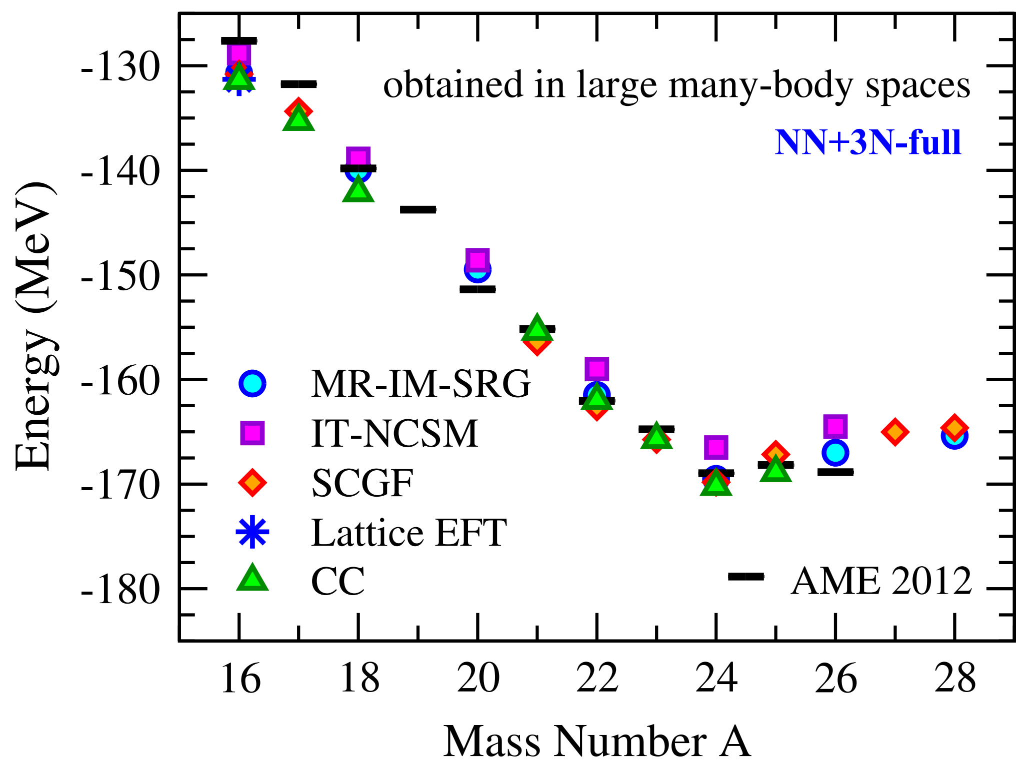
Agreement between all methods with same input forces

No reproduction of dripline in any case

Comparison with Large-Space Methods

Large-space methods with **same SRG-evolved NN+3N-full forces**





Hebeler, JDH, Menéndez, Schwenk, ARNPS (2015)

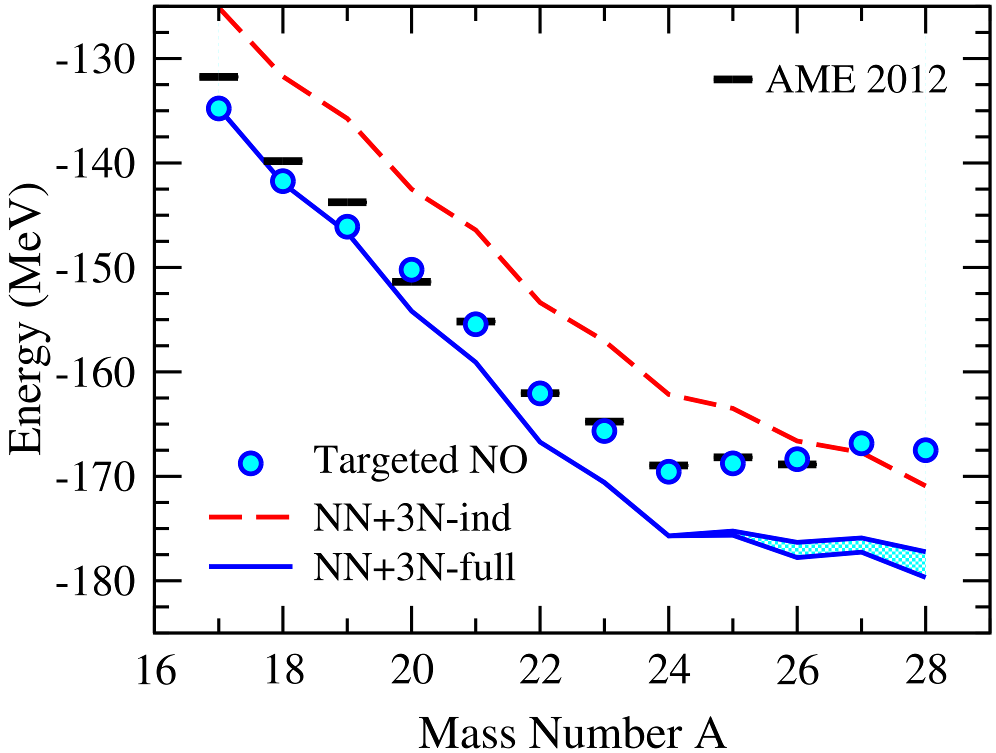
Agreement between all methods with same input forces

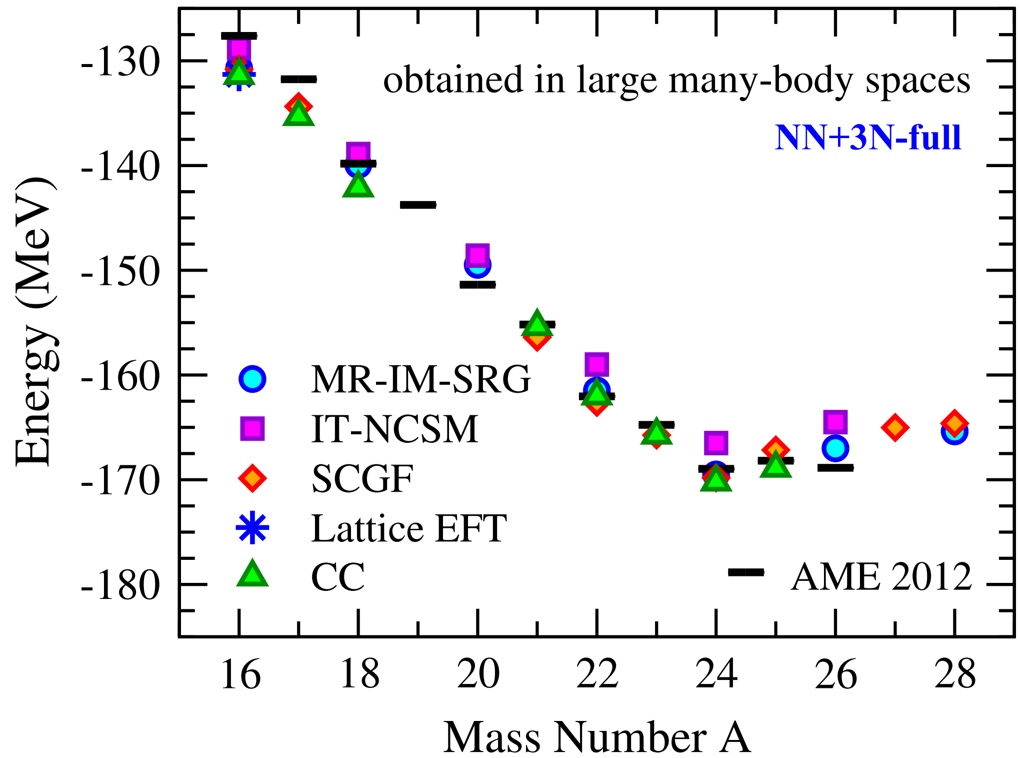
Clear improvement with NN+3N-full

Validates valence-space results

Comparison with Large-Space Methods

Large-space methods with **same SRG-evolved NN+3N-full forces**





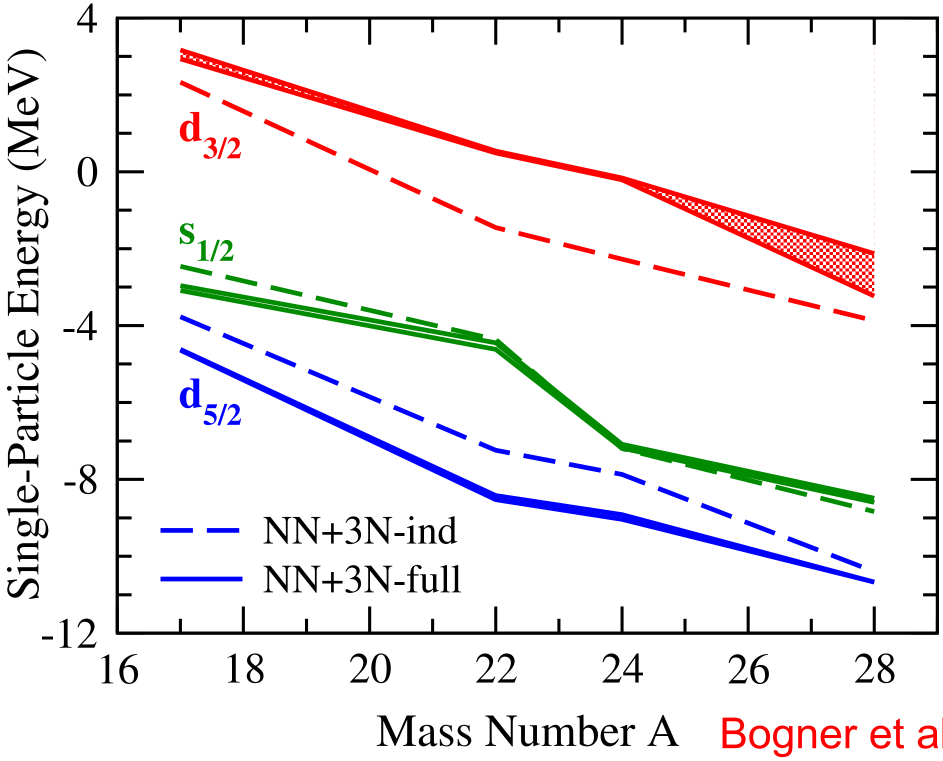
Hebeler, JDH, Menéndez, Schwenk, ARNPS (2015)

Improved method to capture neglected 3N forces in valence space

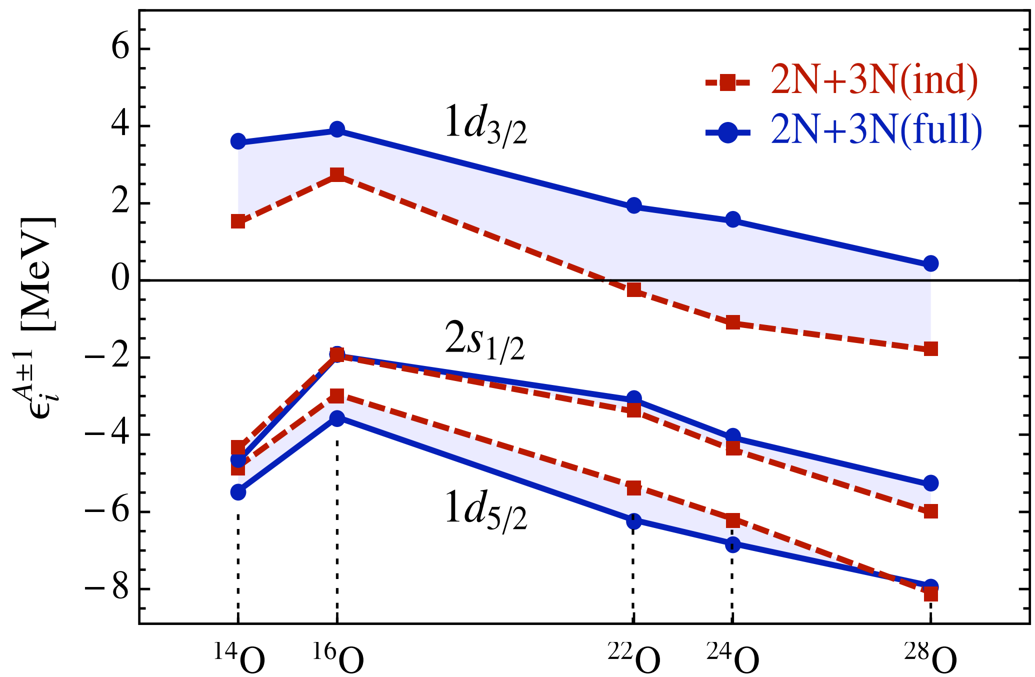
"Targeted" IMSRG results agree well with data and large-scale methods!

Oxygen Dripline Mechanism

Self-consistent Green's Function with **same SRG-evolved NN+3N forces**



Bogner et al., PRL (2014)



Cipollone, Barbieri, Navrátil, PRL (2013)

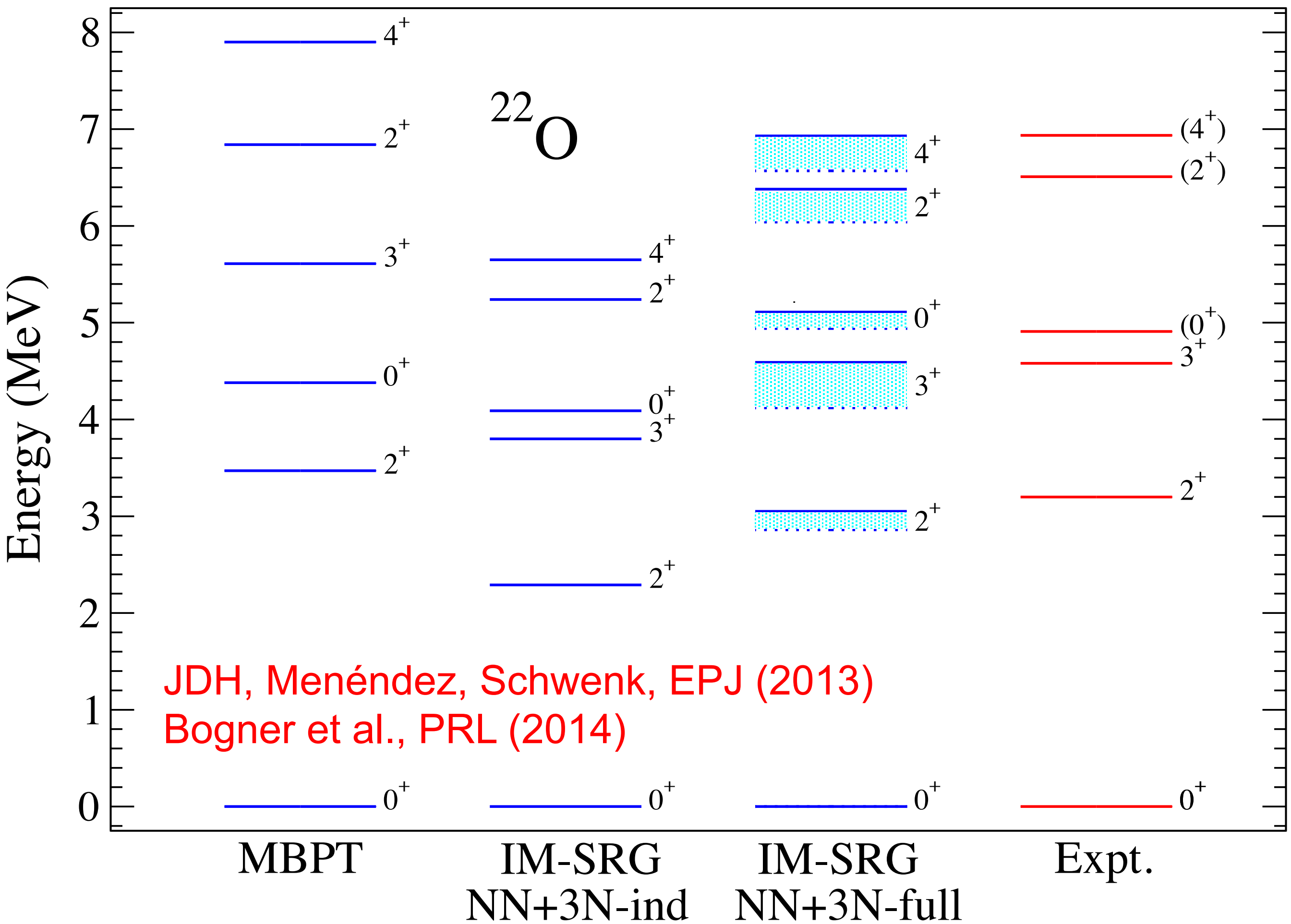
Robust mechanism driving dripline behavior

3N repulsion raises $d_{3/2}$, lessens decrease across shell

Similar to first MBPT NN+3N calculations in oxygen

IM-SRG Oxygen Spectra

Oxygen spectra: extended-space MBPT and *sd*-shell IM-SRG

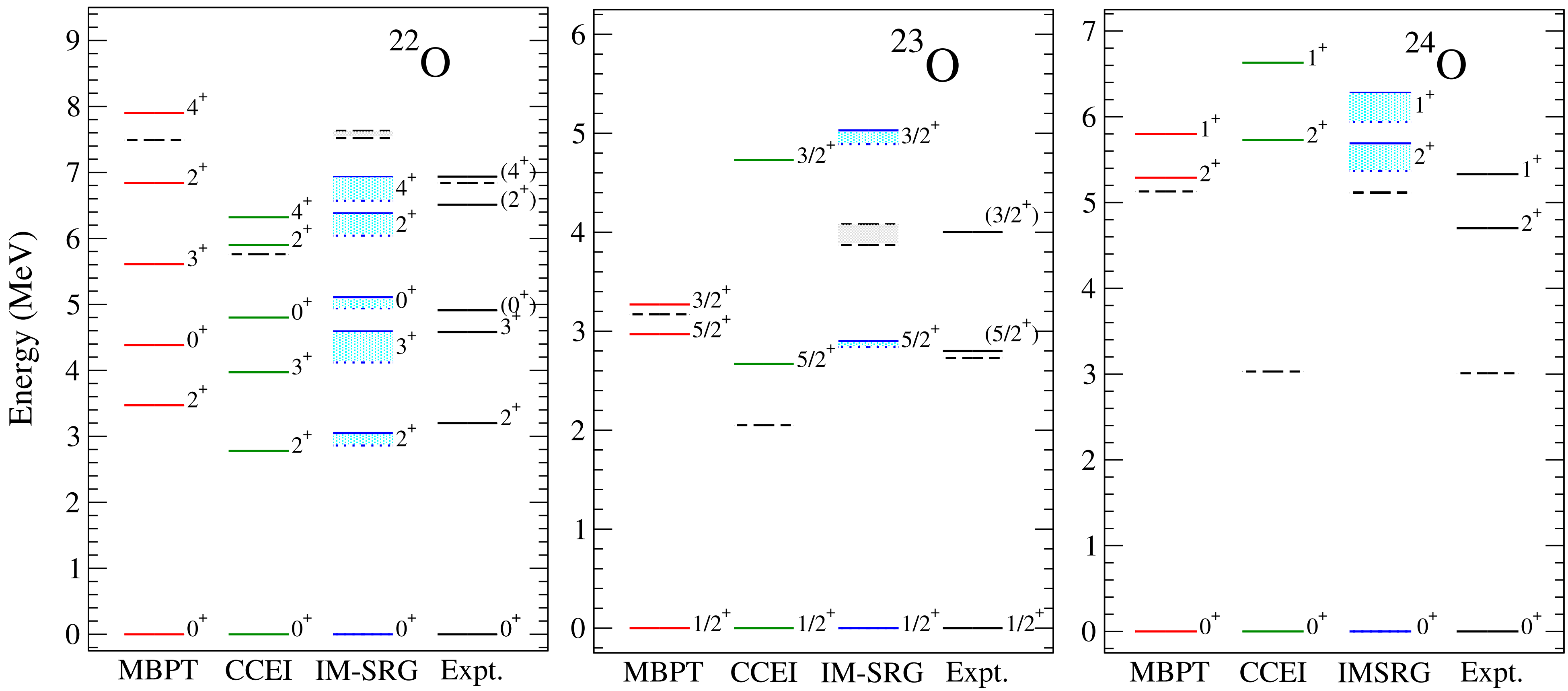


Clear improvement with NN+3N-full

IM-SRG: comparable with phenomenology

Comparison with MBPT/CCEI Oxygen Spectra

Oxygen spectra: Effective interactions from **Coupled-Cluster theory**



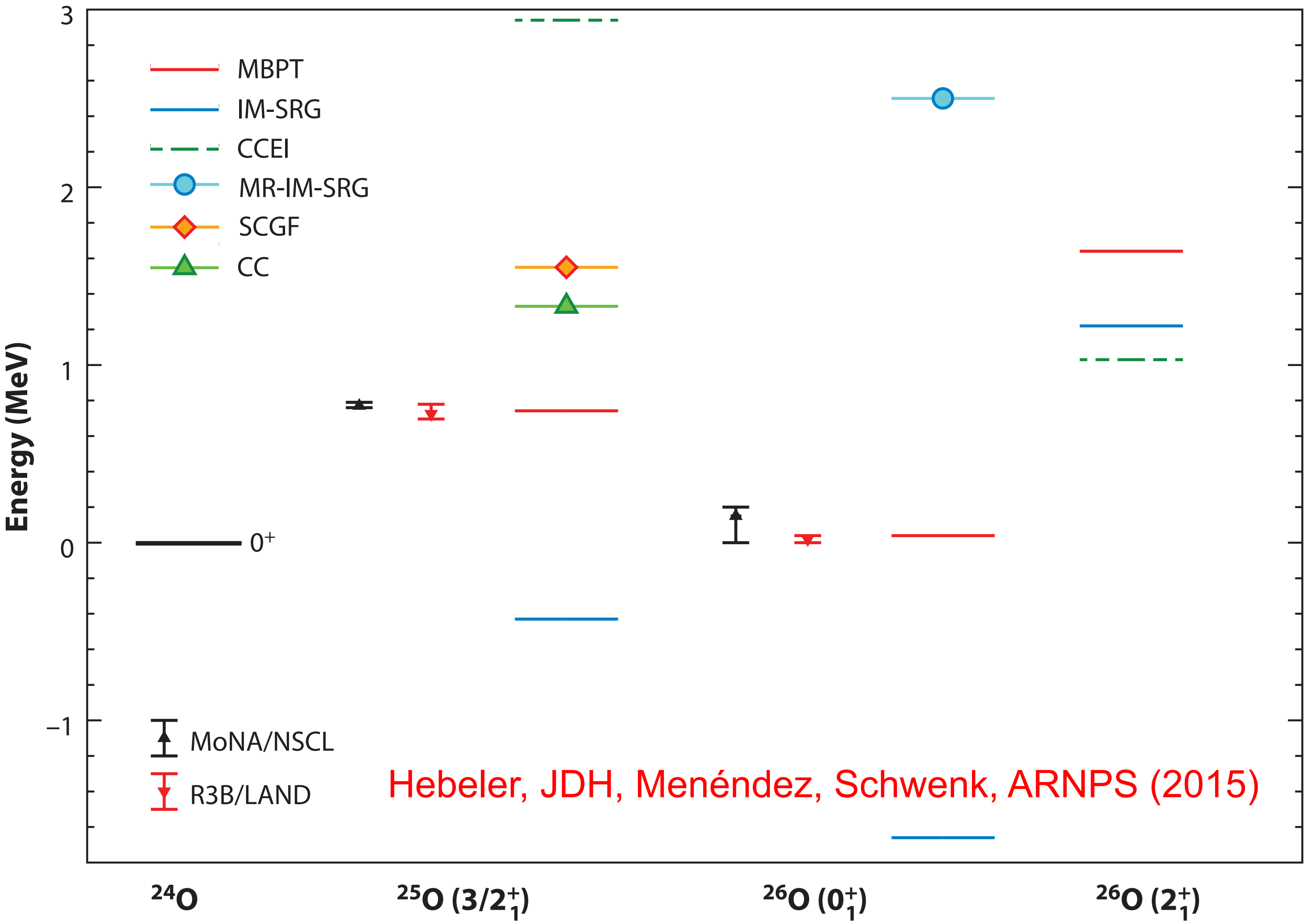
Hebeler, JDH, Menéndez, Schwenk, ARNPS (2015)

MBPT in extended valence space

IM-SRG/**CCEI** spectra agree within ~300 keV

Beyond the Oxygen Dripline

Physics beyond dripline highly sensitive to 3N forces and continuum effects



Prediction of low-lying 2^+ in ^{26}O (recently measured at RIKEN)

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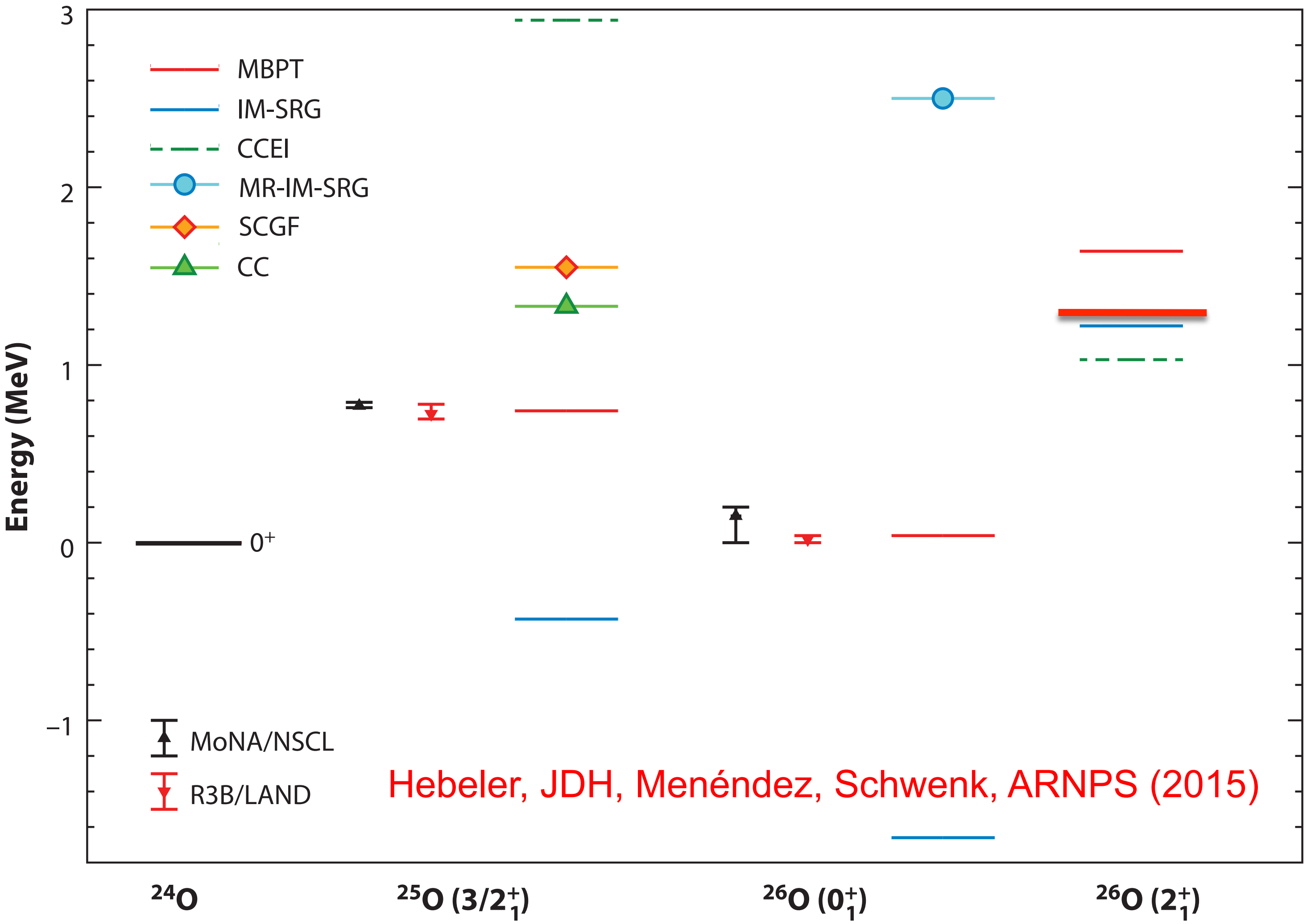
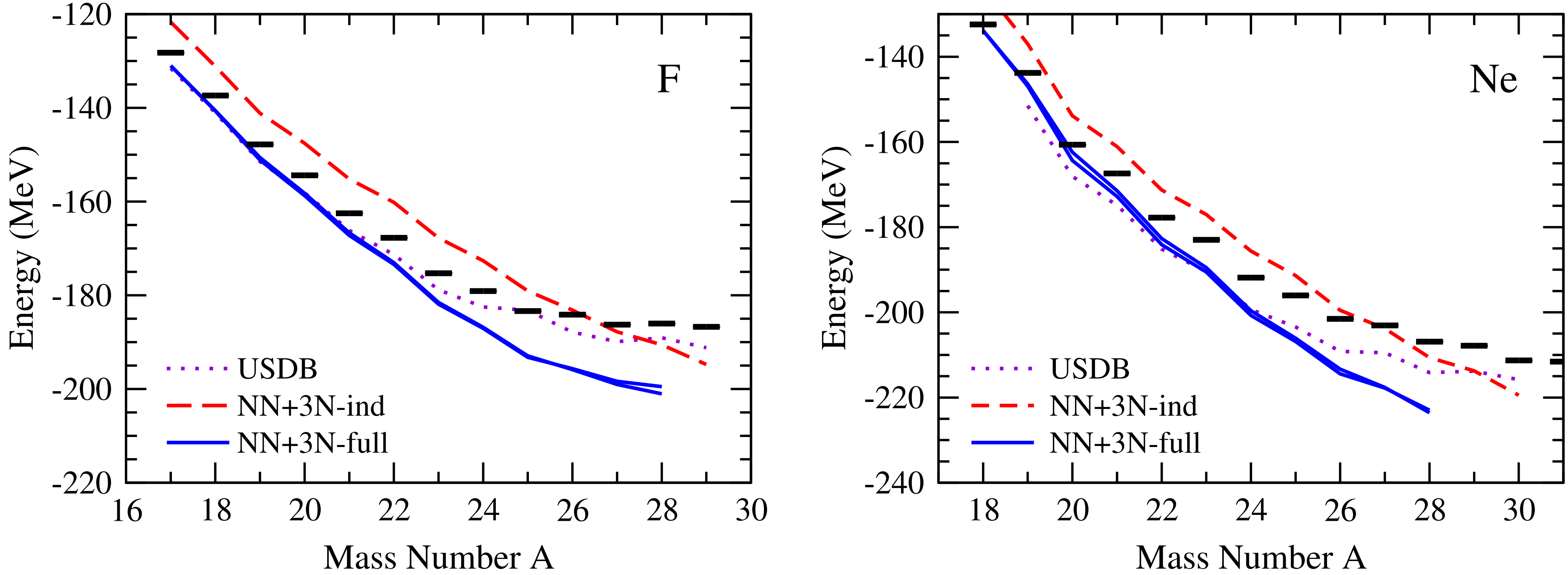


Kondo et al, preliminary

Prediction of low-lying 2^+ in ^{26}O (recently measured at RIKEN)

Beyond Semi-Magic: Ground-States of F/Ne

IM-SRG valence-space results for fully open F/Ne isotopes



Bogner, Hergert, JDH, Schwenk, Stroberg, in prep.

NN+3N-ind incorrect trend

NN+3N-full improved agreement with experiment; overbound past N=14

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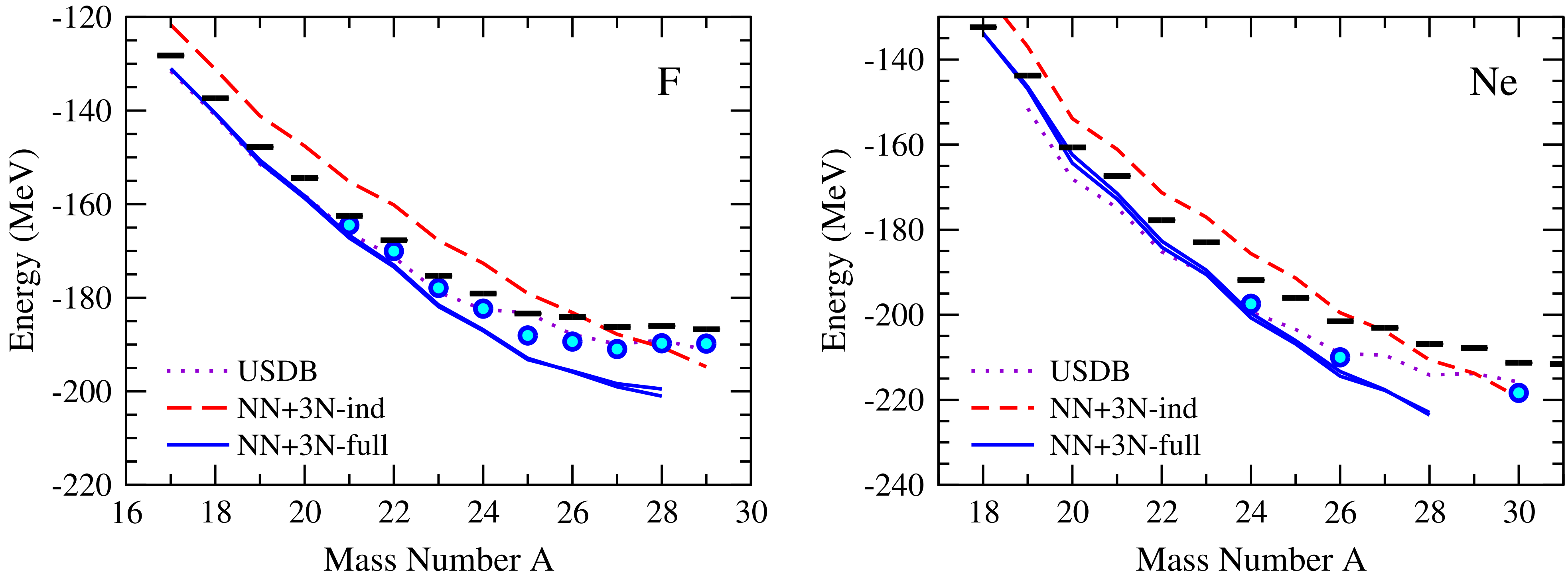

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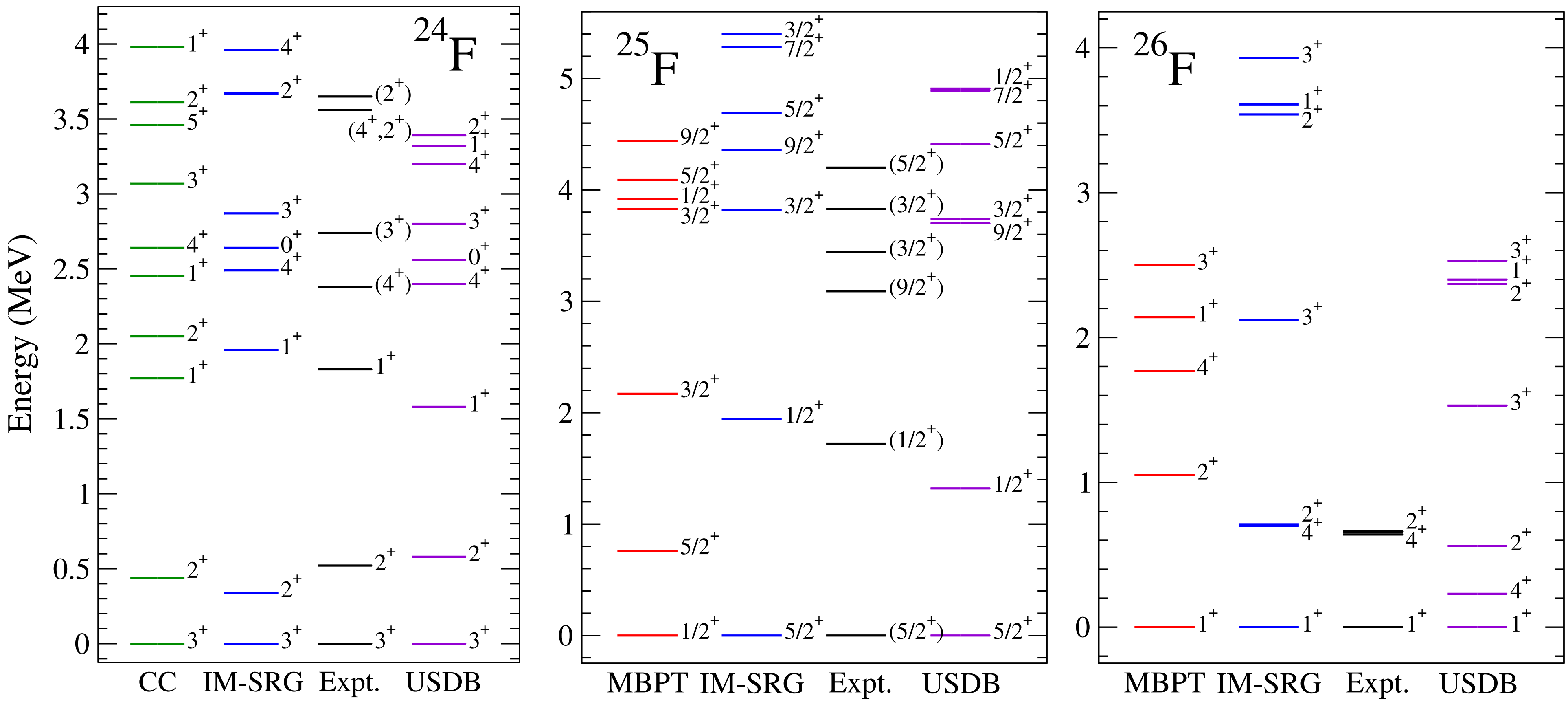
NN+3N-ind incorrect trend

NN+3N-full improved agreement with experiment; overbound past N=14

“Targeted” normal ordering gives results very similar to phenomenology

Fully Open Shell: Neutron-Rich Fluorine Spectra

Fluorine spectroscopy: **MBPT** and **IM-SRG** (*sd* shell) from NN+3N forces



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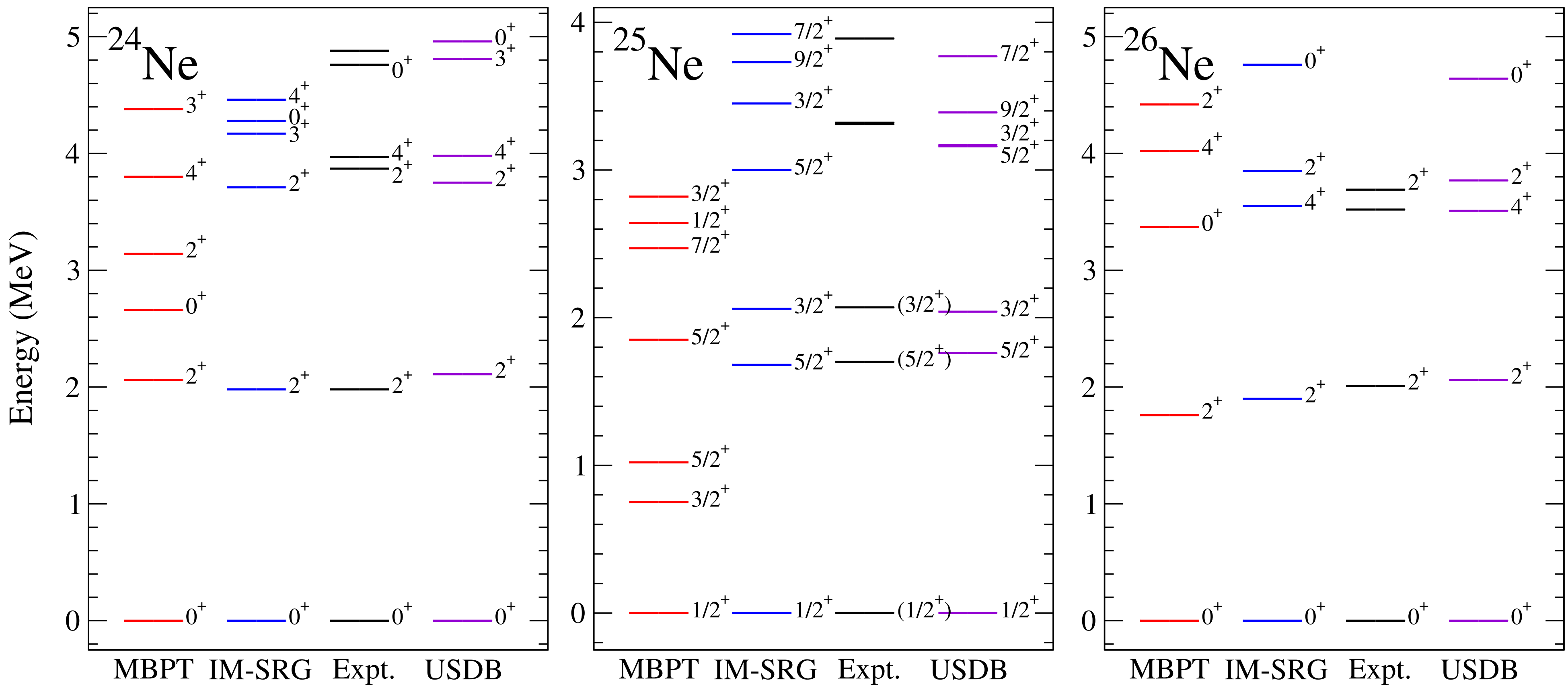
IM-SRG: **competitive with phenomenology**, good agreement with data

Fully Open Shell: Neutron-Rich Neon Spectra

Neon spectra: extended-space MBPT and IM-SRG (*sd* shell)



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MBPT: clear deficiencies

IM-SRG: **competitive with phenomenology**, good agreement with data

Alternative Approach: Magnus Expansion

Morris, **Parzuchowski**, Bogner, arXiv:1507.06725

Magnus expansion: ***explicitly*** construct unitary transformation

$$U(s) = \exp \Omega(s)$$

With flow equation:

$$\frac{\mathrm{d}\Omega(s)}{\mathrm{d}s} = \eta(s) + \frac{1}{2}\left[\Omega(s), \eta(s)\right] + \frac{1}{12}\left[\Omega(s), \left[\Omega(s), \eta(s)\right]\right] + \ldots$$

Leads to commutator expression for evolved Hamiltonian

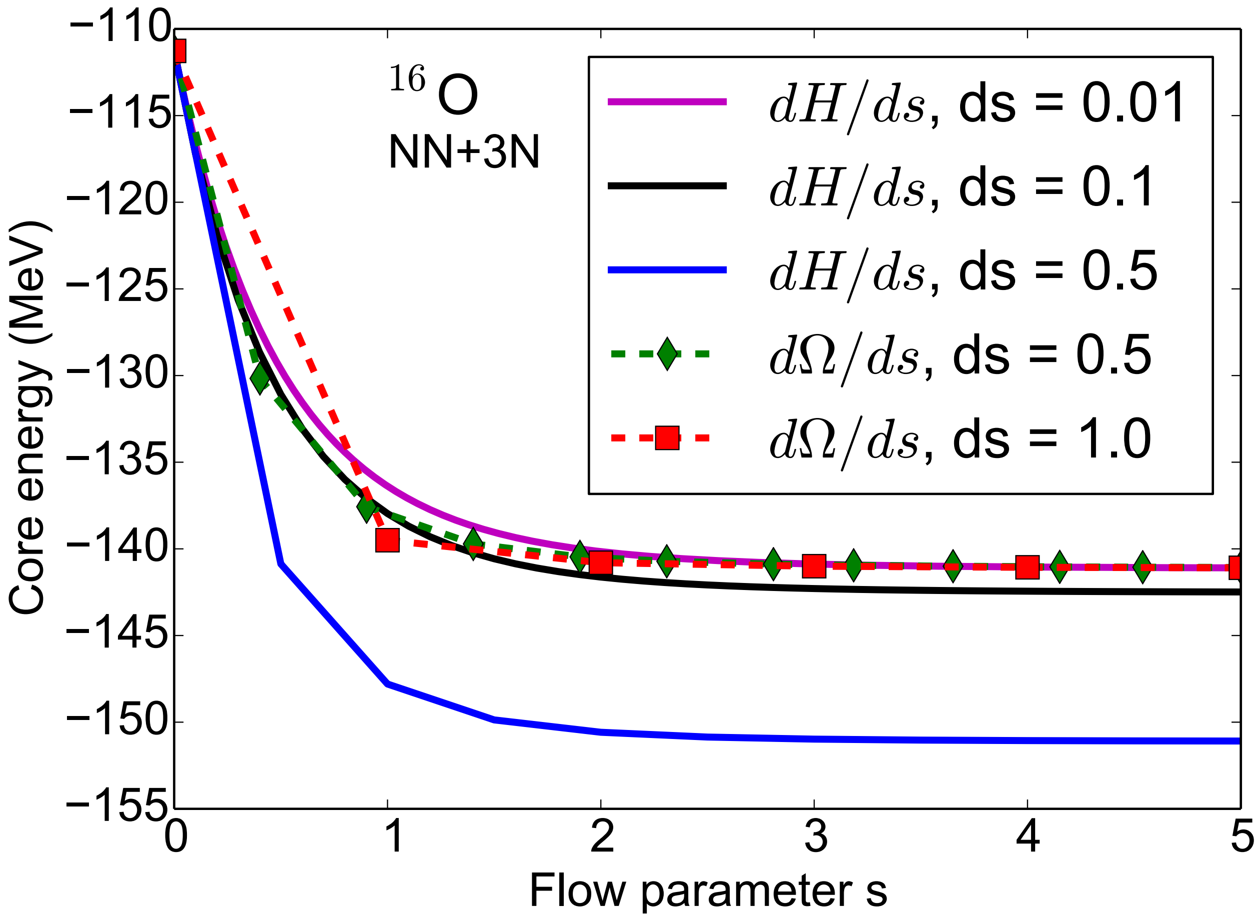
$$H(s) = e^{\Omega(s)} H e^{-\Omega(s)} = H + \frac{1}{2}\left[\Omega(s), H\right] + \frac{1}{12}\left[\Omega(s), \left[\Omega(s), H\right]\right] + \cdots$$

Nested commutator series – in practice truncate numerically

All calculations truncated at normal-ordered two-body level

Magnus vs Flow-Equation

Variation of step size



Evident error accumulation in flow-equation for small step sizes

Magnus: rapid convergence, independent of step size

Effective Operators

Keep unitary transformation from evolution of Hamiltonian

Can generalize to arbitrary operators

$$H(s) = e^{\Omega(s)} H e^{-\Omega(s)} = H + \frac{1}{2}\left[\Omega(s), H\right] + \frac{1}{12}\left[\Omega(s), \left[\Omega(s), H\right]\right] + \cdots$$

$$\Downarrow$$

$$\mathcal{O}^{\Lambda}(s) = e^{\Omega(s)} \mathcal{O}^{\Lambda} e^{-\Omega(s)} = \mathcal{O}^{\Lambda} + \frac{1}{2}\left[\Omega(s), \mathcal{O}^{\Lambda}\right] + \frac{1}{12}\left[\Omega(s), \left[\Omega(s), \mathcal{O}^{\Lambda}\right]\right] + \cdots$$

Must work out normal-ordered operators in *J*-coupled basis

First apply to scalar operators

E0 Transitions and Radii

Seldom calculated in nuclear shell model

In single HO shell:

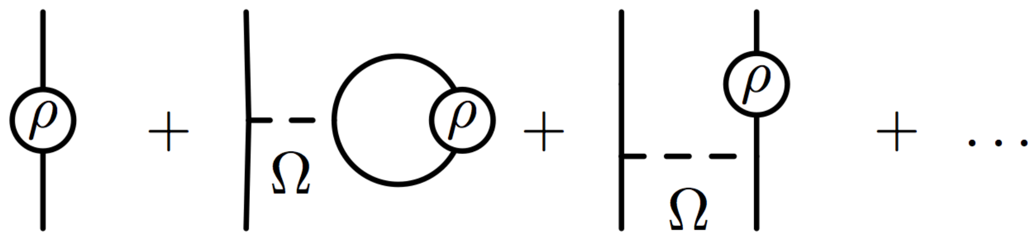
$$|\langle f|\rho_{E0}|i\rangle|^2 \propto \delta_{ij} \text{ where } \rho_{E0} = \frac{1}{e^2 R}\sum_i e_i r_i^2$$

Must resort to other methods

IM-SRG: straightforward to calculate effective valence-space operator:

$$\rho_{E0}(s) = e^{\Omega(s)}\rho_{E0}e^{-\Omega(s)} = \rho_{E0} + \frac{1}{2}\left[\Omega(s), \rho_{E0}\right] + \cdots$$

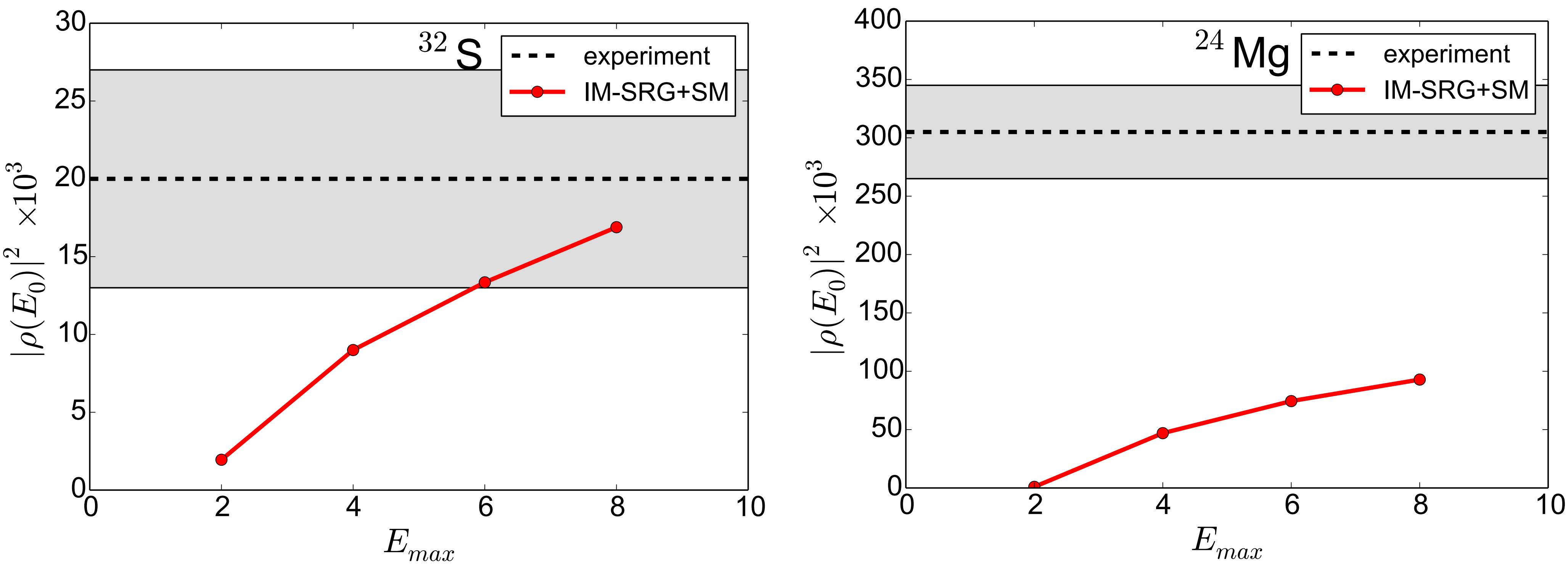
Commutators induce important higher-order and two-body parts



Quantify importance of induced higher-body contributions!

E0 Transitions in sd Shell Model

Preliminary results in *sd* shell:

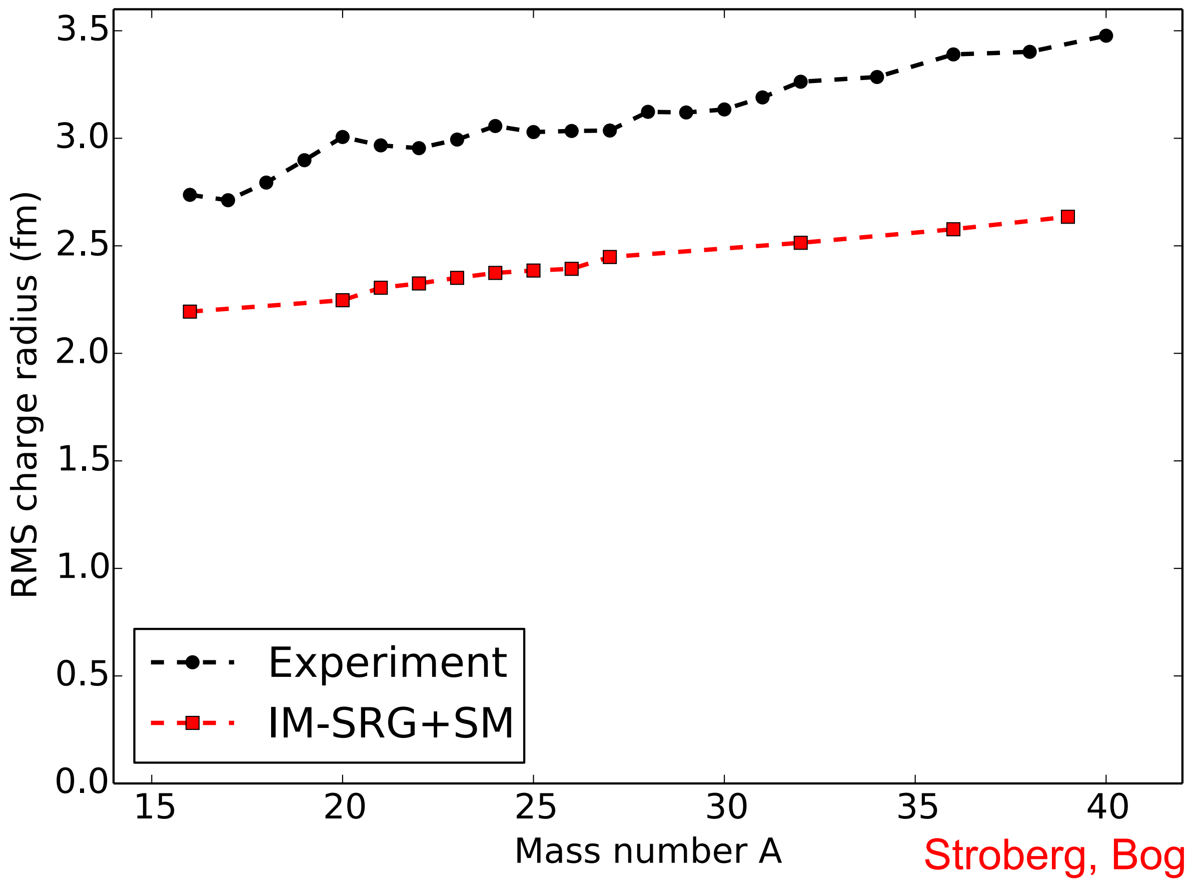


Promising but need additional benchmarks

RMS Charge Radii in sd Shell Model

Previous SM radii calculations rely on empirical input or as relative to core

Absolute radii for entire sd shell calculated in shell model NN+3N



Stroberg, Bogner, Hergert, JDH, Schwenk , in prep

Benchmarked against NCSM in various SM codes

~10% too small – deficiencies expected to come from initial Hamiltonian

Two-body part important 15-20%

New Directions and Outlook

Heavier semi-magic chains: MBPT as guide

Ab initio valence-shell Hamiltonians

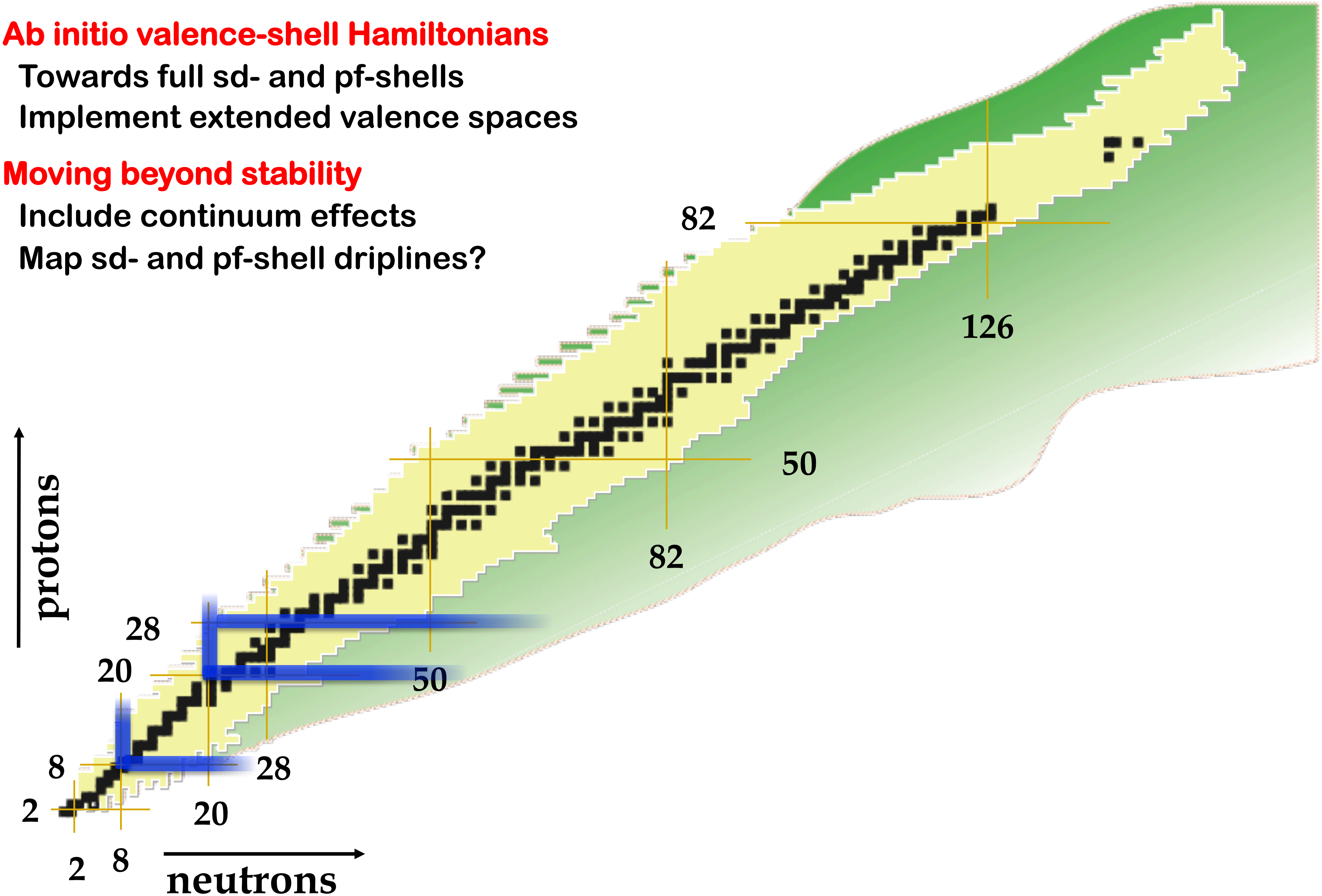
Towards full sd- and pf-shells

Implement extended valence spaces

Moving beyond stability

Include continuum effects

Map sd- and pf-shell driplines?



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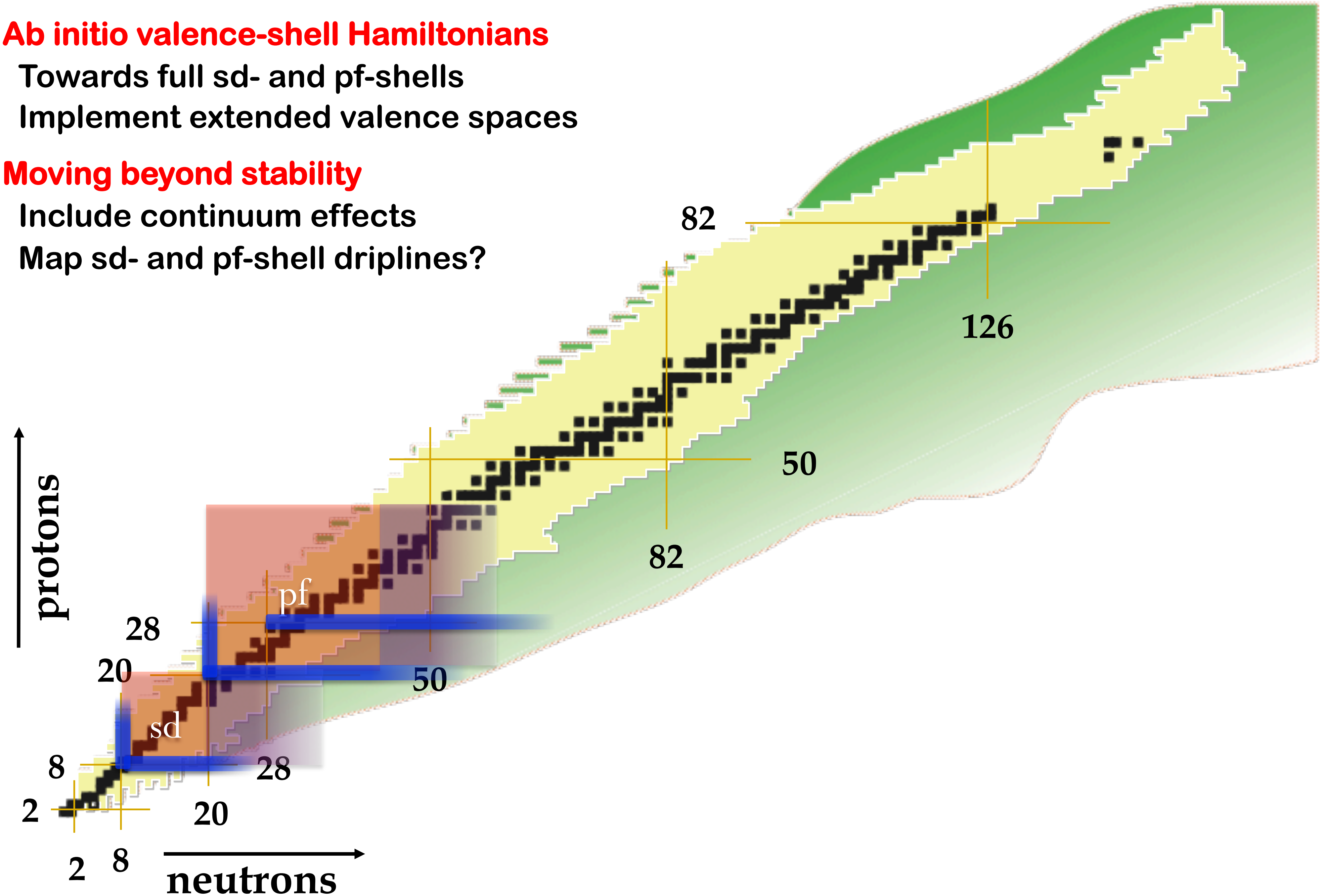

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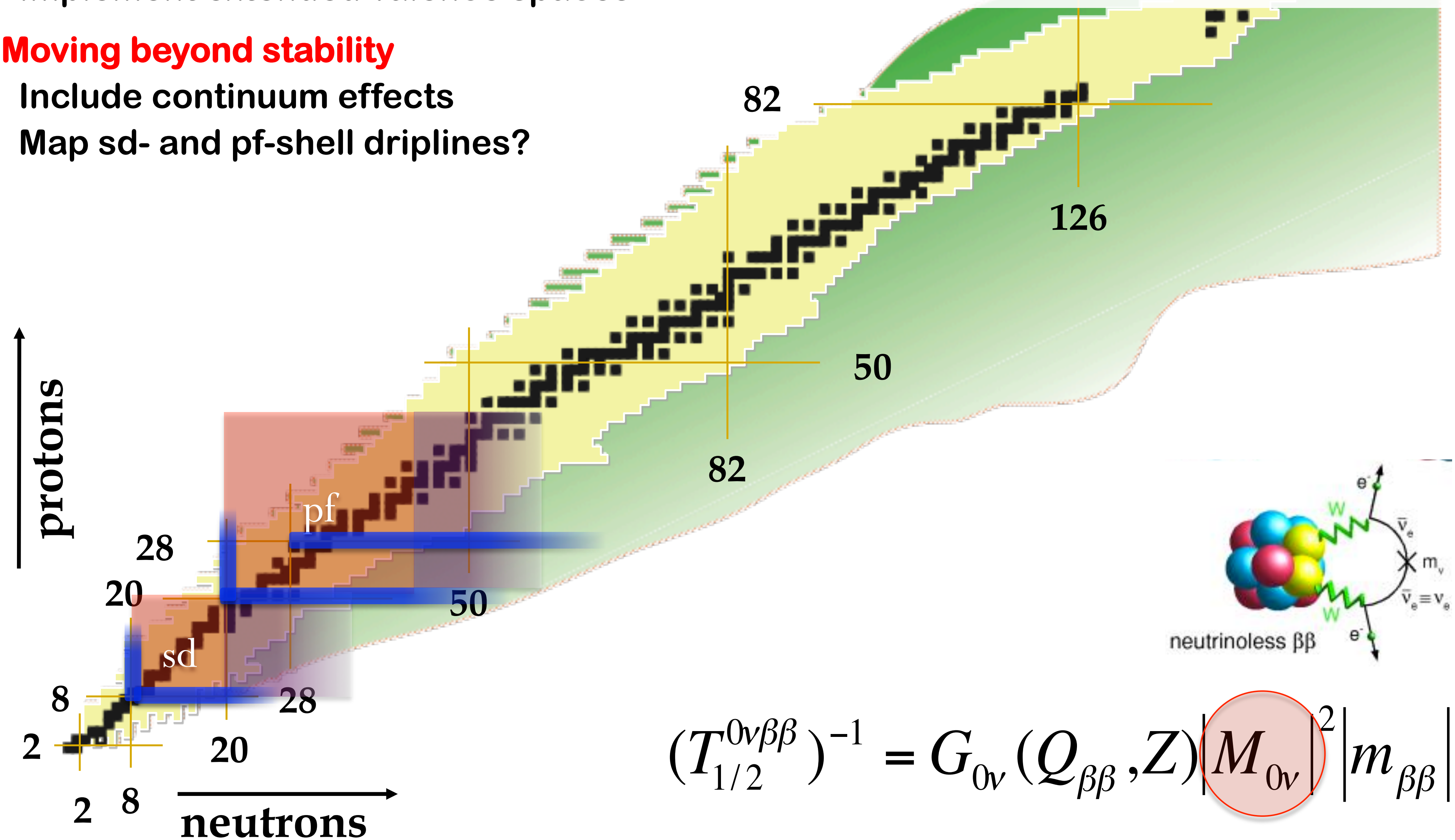
Map sd- and pf-shell driplines?

Fundamental symmetries

Effective electroweak operators

Non-empirical calculation of $0\nu\beta\beta$ decay

WIMP-nucleus scattering



$$(T_{1/2}^{0\nu\beta\beta})^{-1} = G_{0\nu}(Q_{\beta\beta}, Z)\left|M_{0\nu}\right|^2 \left|m_{\beta\beta}\right|^2$$