# Nonperturbative Shell-Model Interactions from In-Medium SRG

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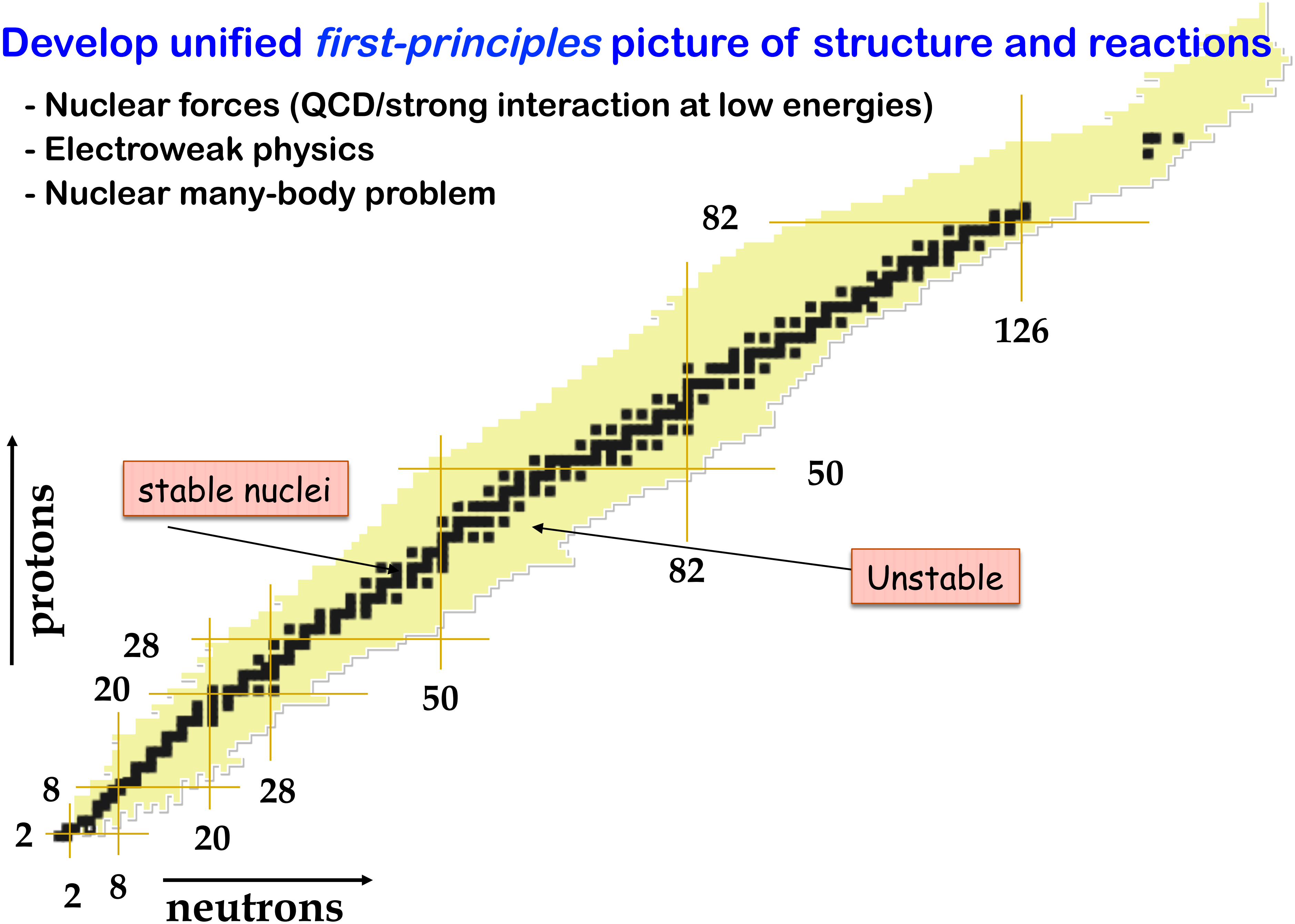
# Frontiers and Impact of Nuclear Science

**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

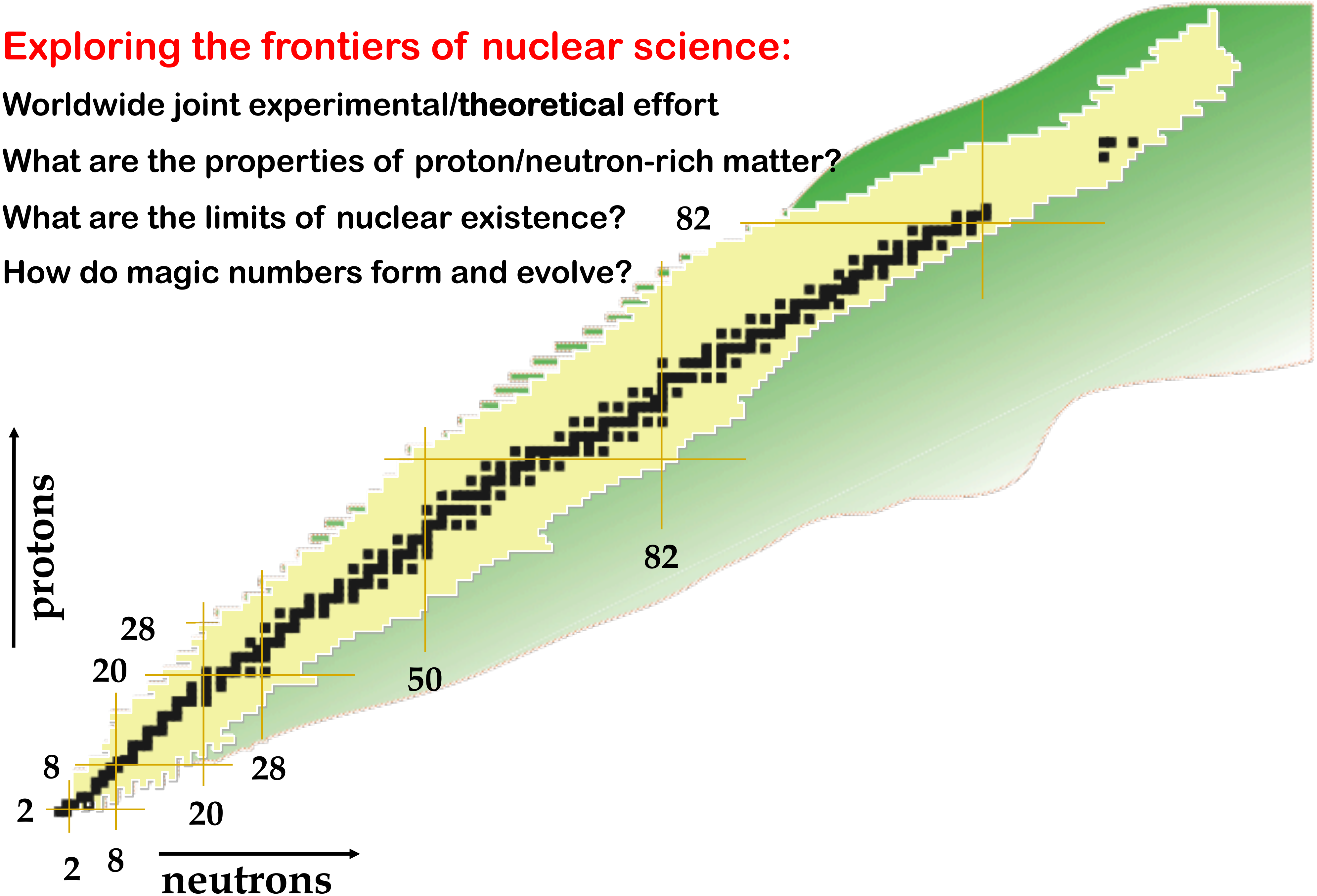
## Exploring the frontiers of nuclear science:

**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?**



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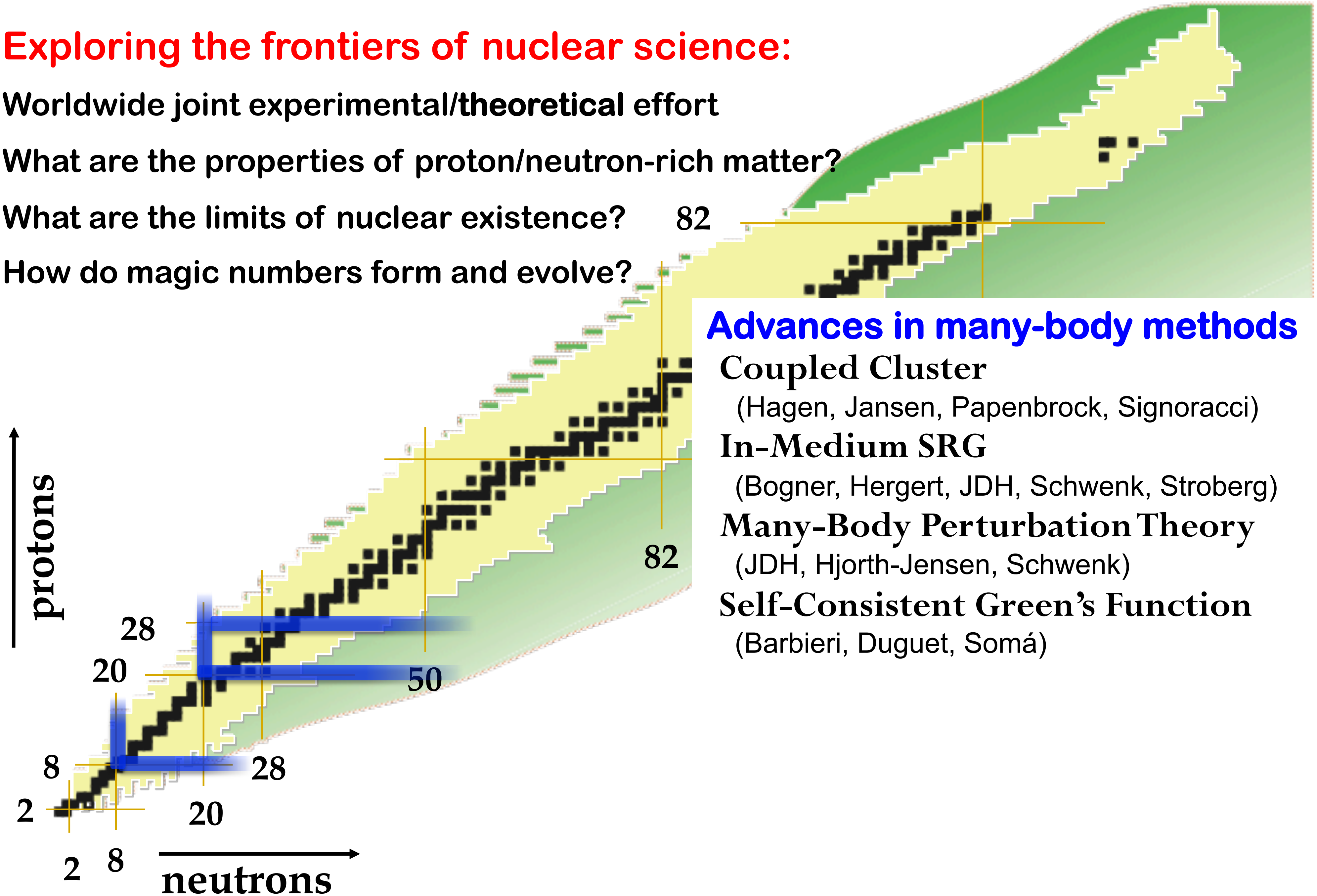


### Advances in many-body methods

**Coupled Cluster**
(Hagen, Jansen, Papenbrock, Signoracci)

**In-Medium SRG**
(Bogner, Hergert, JDH, Schwenk, Stroberg)

**Many-Body Perturbation Theory**
(JDH, Hjorth-Jensen, Schwenk)

**Self-Consistent Green's Function**
(Barbieri, Duguet, Somá)

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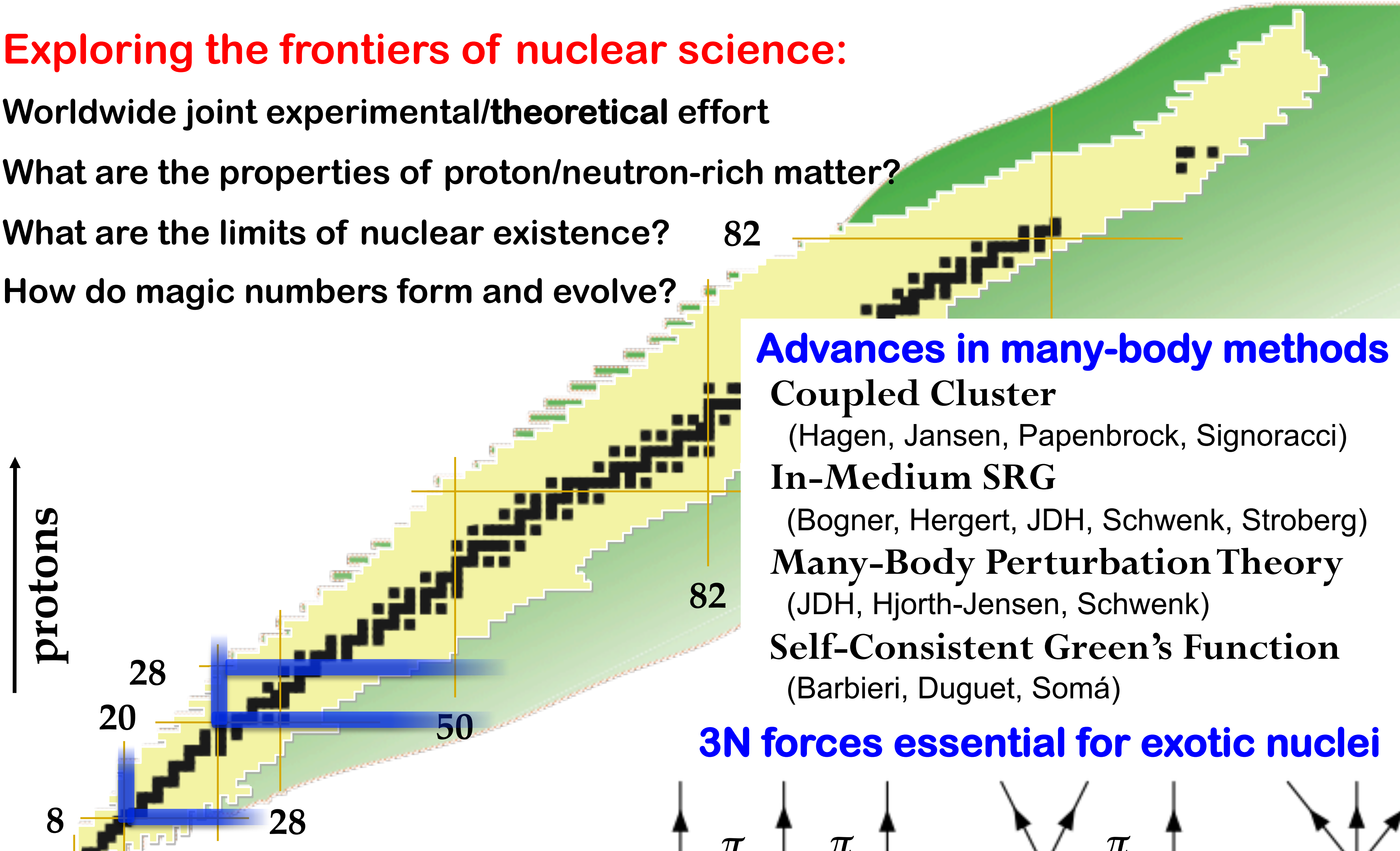


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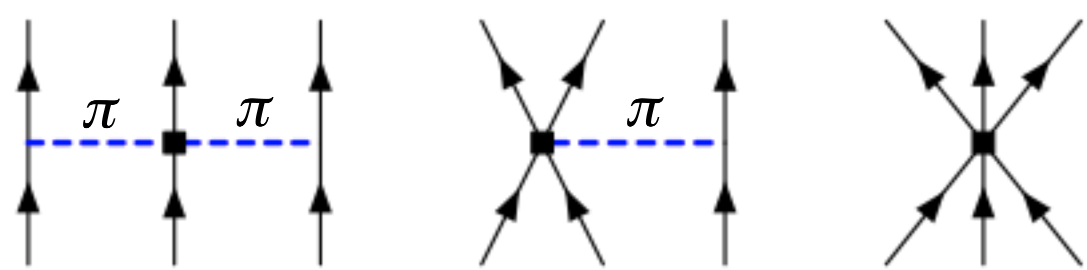
### 3N forces essential for exotic nuclei



# The Nuclear Many-Body Problem

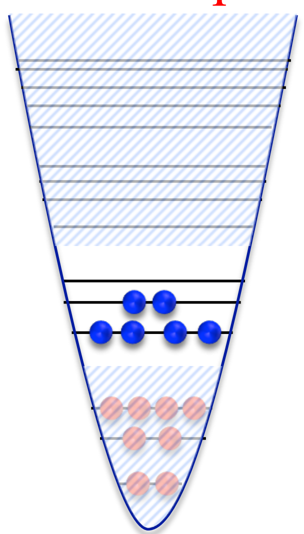
Nucleus strongly interacting many-body system – how to solve $A$-body problem?

$$H\psi_n = E_n\psi_n$$

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

**Large scale**: controlled approximations to solving full Schrödinger Equation

Medium-mass
Valence space

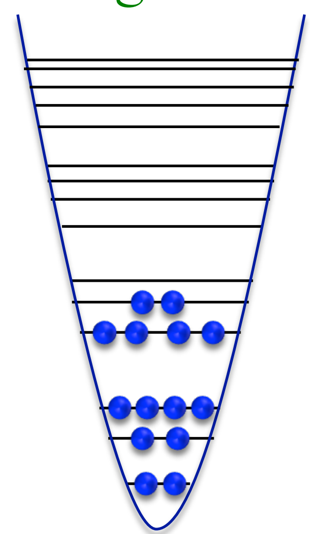


Any nuclei near closed shell cores

All properties:
- Ground states
- Excited states
- EW transitions

**Coupled Cluster**
**In-Medium SRG**
**Perturbation Theory**

Medium-mass
Large scale



Limited range:
- Closed shell $\pm 1$
- Even-even

Limited properties:
- Ground states only
- Some excited state

**Coupled Cluster**
**In-Medium SRG**
**Green's Function**

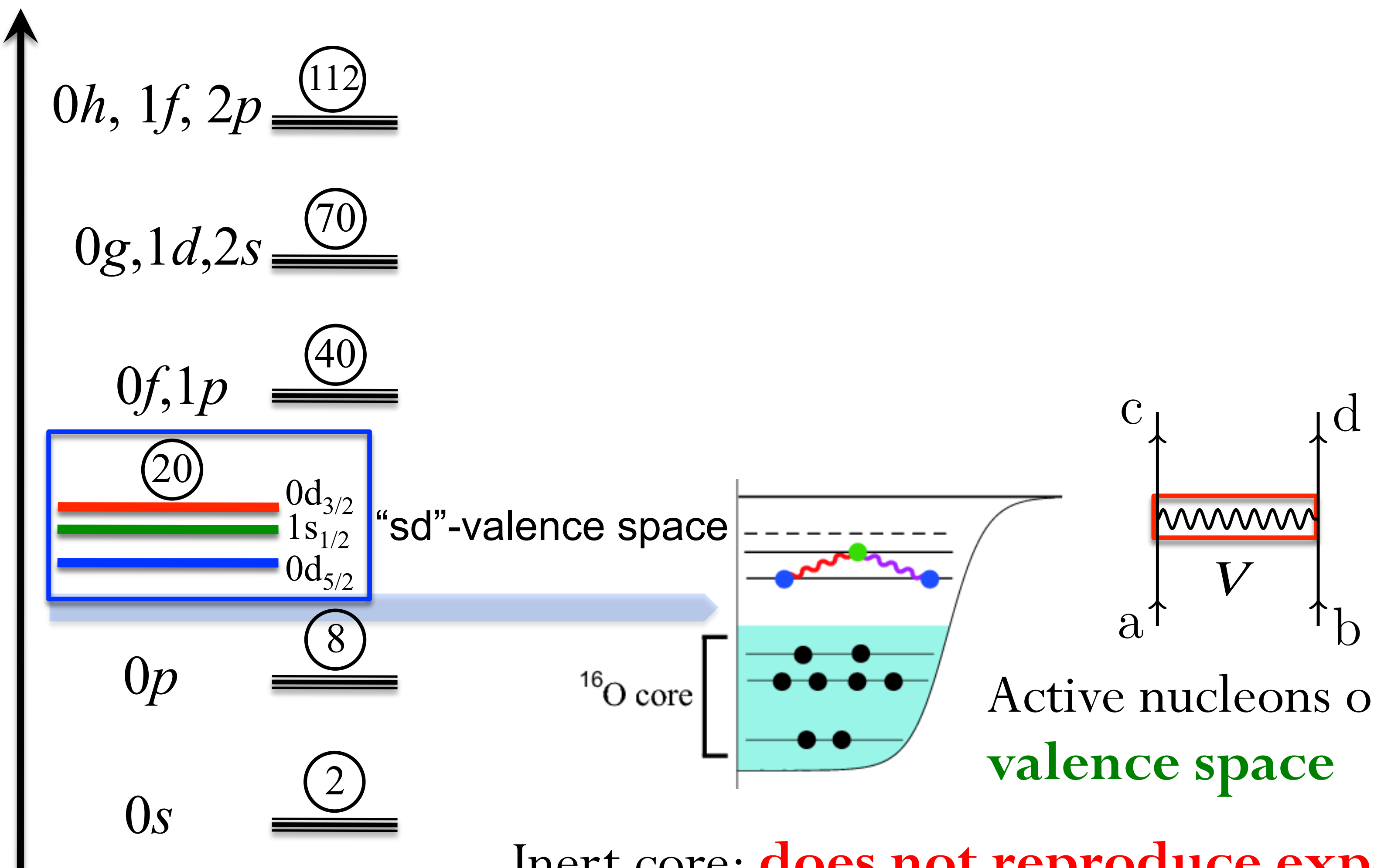
# Valence-Space Ideas

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

Calculate **valence-space** Hamiltonian inputs from nuclear forces

**Interaction matrix elements**

**Single-particle energies (SPEs)**




Active nucleons occupy **valence space**

Inert core: **does not reproduce experiment**

# Valence-Space Ideas

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

Calculate **valence-space** Hamiltonian inputs from nuclear forces

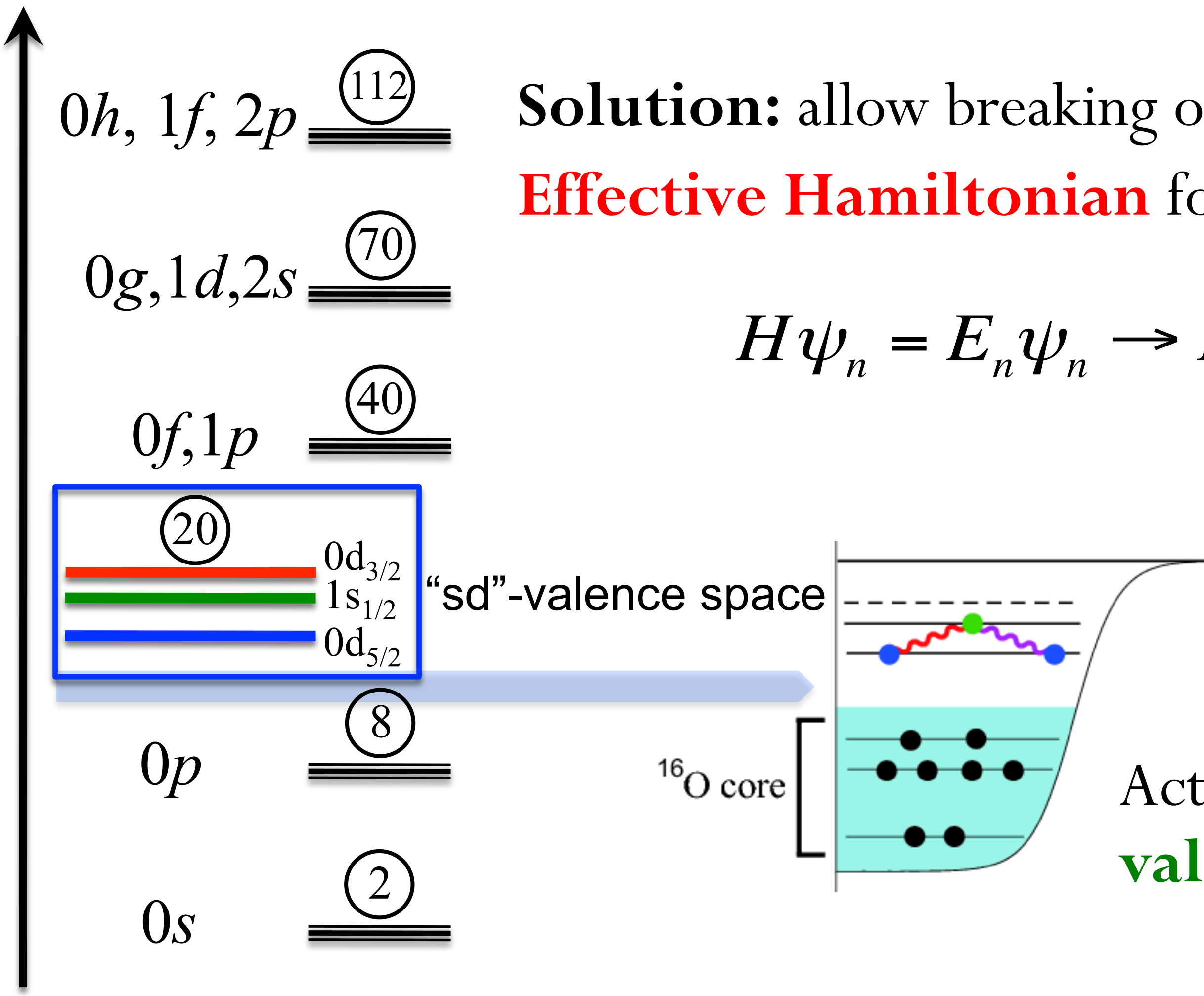
**Interaction matrix elements**

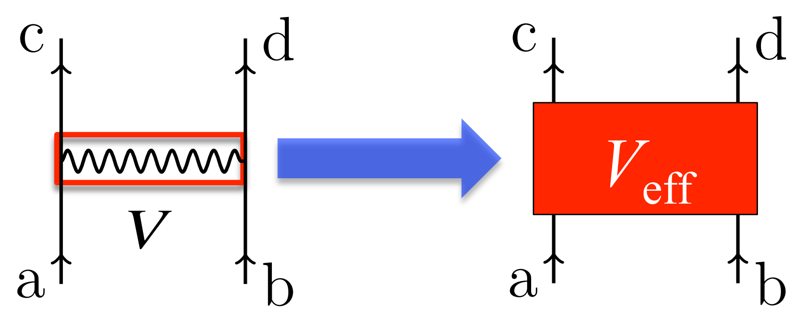
**Single-particle energies (SPEs)**

**Solution:** allow breaking of core

**Effective Hamiltonian** for valence nucleons

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




Active nucleons occupy **valence space**

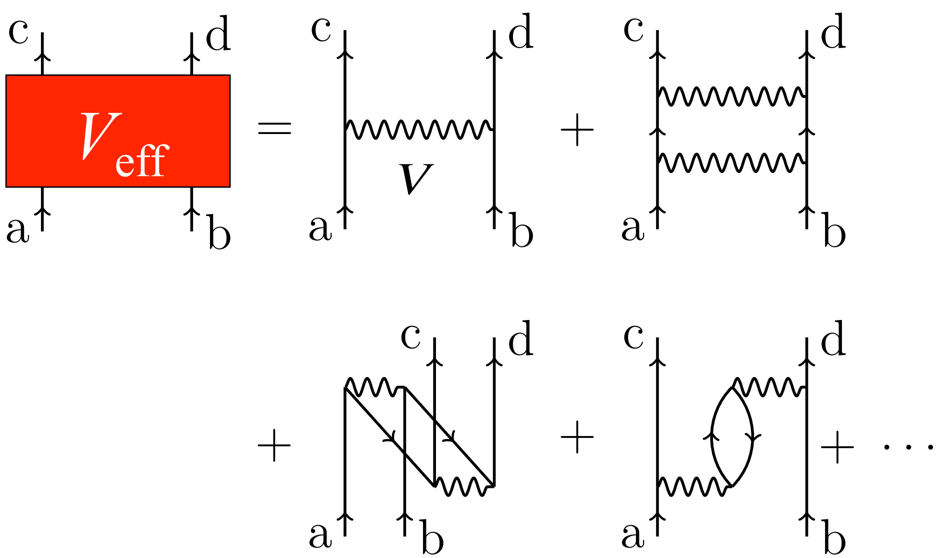
# Perturbative Approach

1) Effective interaction: sum excitations outside valence space to **3$^{rd}$ order**

2) Single-particle energies calculated self consistently

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

4) NN and 3N forces from chiral EFT – to 3$^{rd}$-order MBPT



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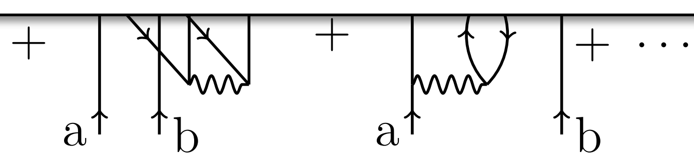
<u>Limitations</u>

- 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)



# Perturbative Approach

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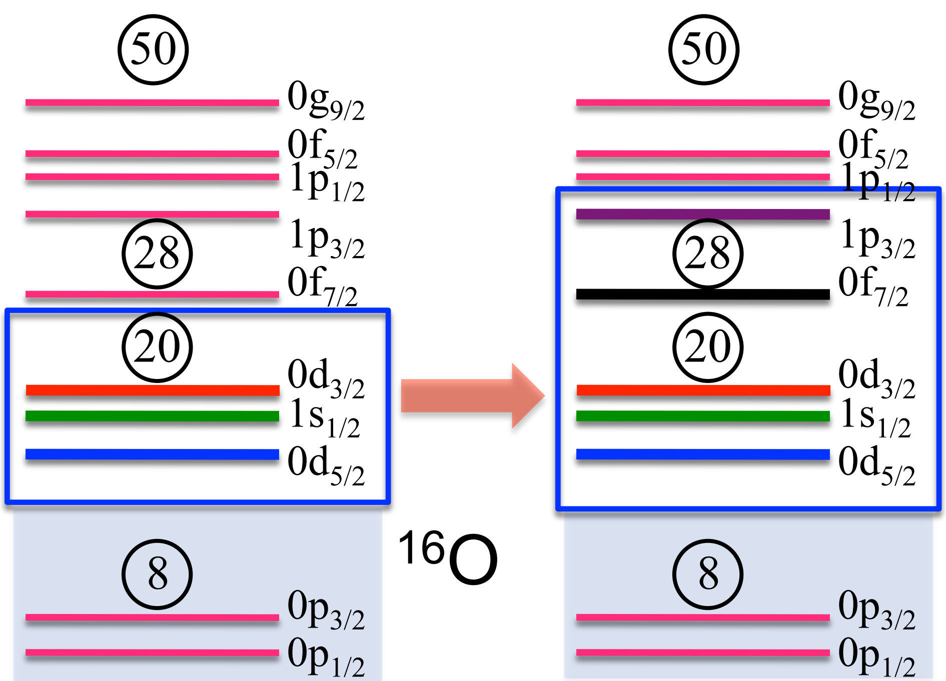
3) Harmonic-oscillator basis of 13-15 major shells: **converged**

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

5) Need **extended valence spaces**

**Philosophy**: diagonalize in largest possible valence space (where orbits relevant)

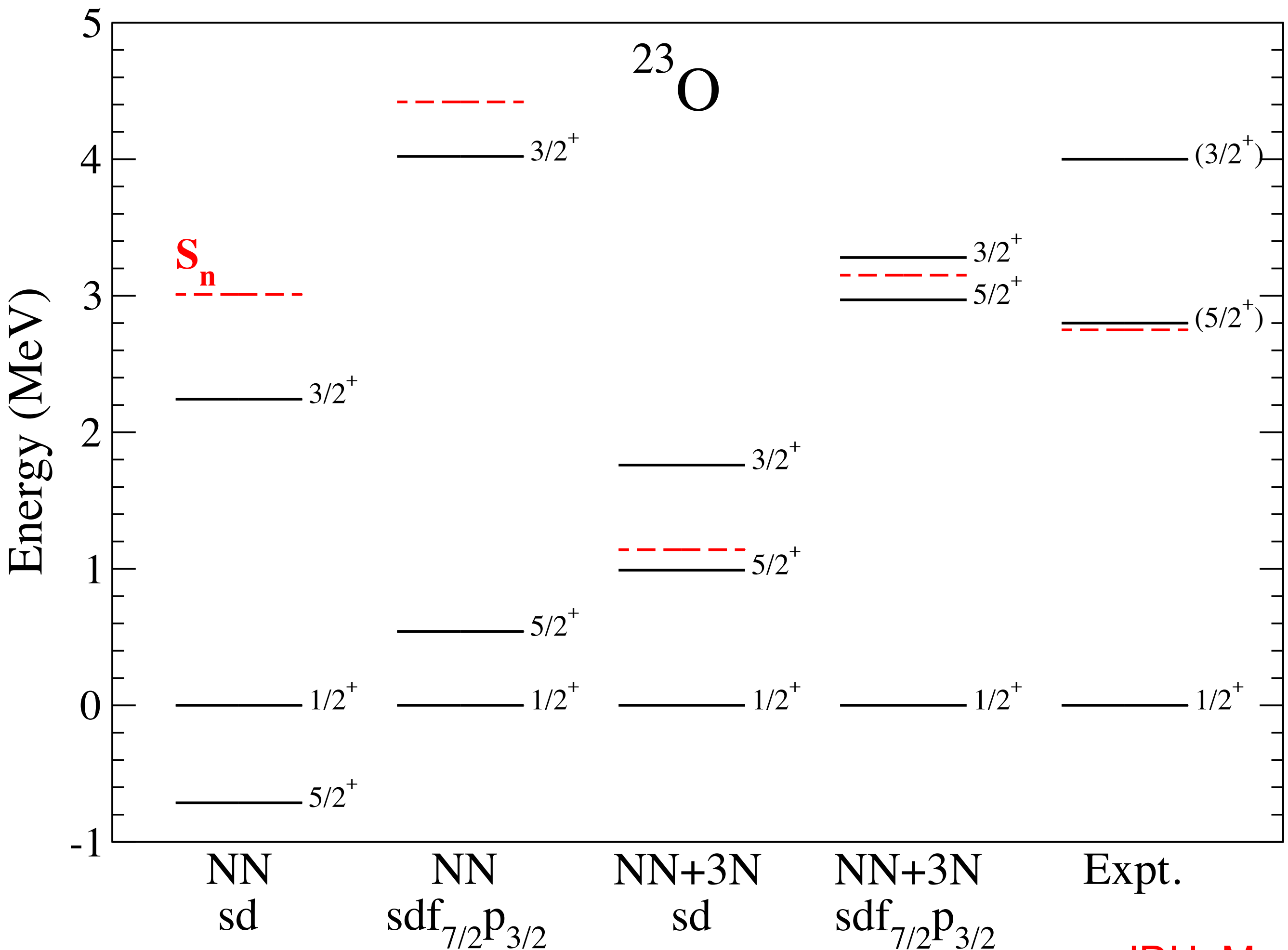



Treats higher orbits nonperturbatively

# 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, Menendez, Schwenk, EPJA (2013)

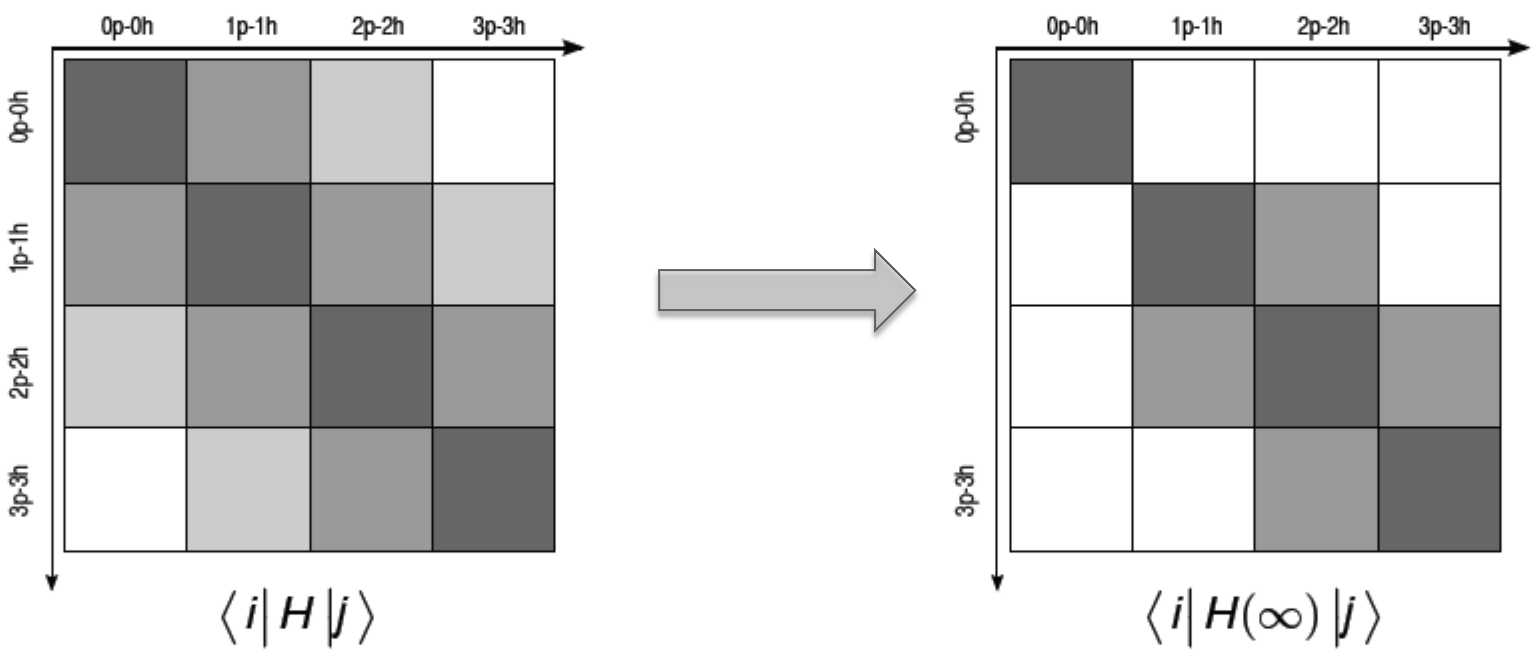
# Nonperturbative In-Medium SRG: Reminder

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

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

Tsukiyama, Bogner, Schwenk, PRL (2011)

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



# Flow Equation Formulation

**Flow equation:** define *U(s)* implicitly with particular choice of generator

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

chosen for desired decoupling behavior (Wegner, White, Im. Time, etc)

Solving flow equation (Hamiltonian and generator truncated at 2-body level)

$$\frac{\mathrm{d}H(s)}{\mathrm{d}s} = \left[\eta(s), H(s)\right]$$

Drives all n-particle n-hole couplings to 0 for **closed-shell reference state**

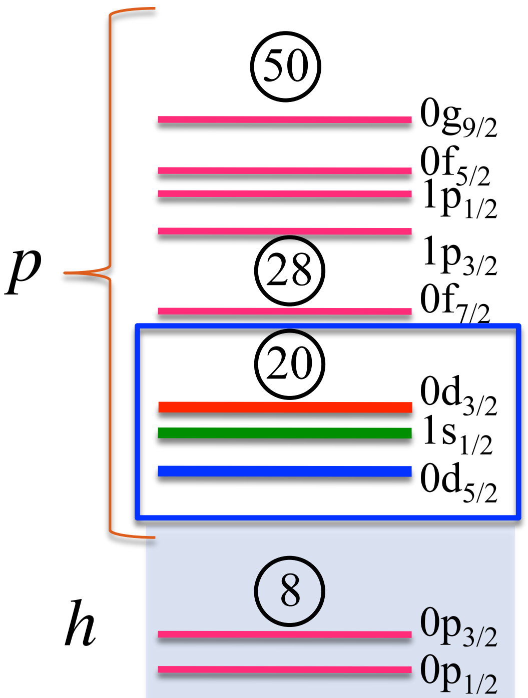
$$\langle npnh | H(\infty) | \Phi_c \rangle = 0$$

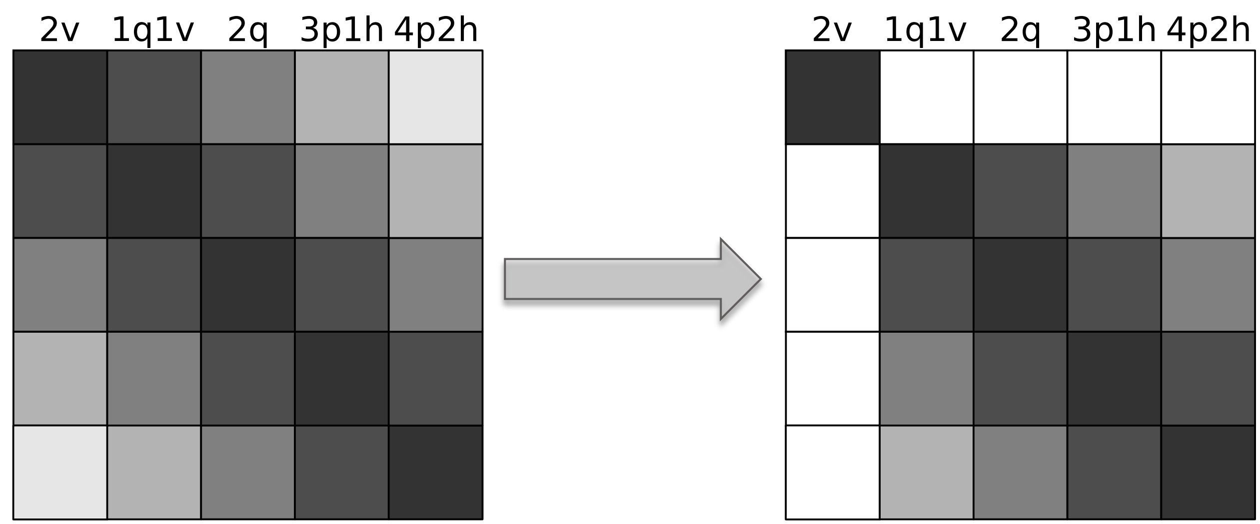
# IM-SRG: Valence-Space Formulation

**Open shell systems** Tsukiyama, Bogner, Schwenk, PRC (2012)

Split particle states into valence states, $v$, and those above valence space, $q$

Redefine "off-diagonal" to include excitations of valence particles outside v.s.




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

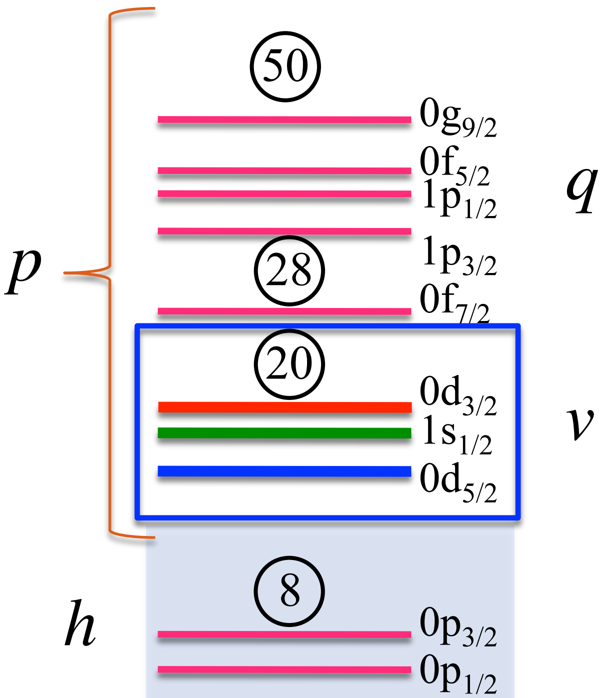
$$H^{\mathrm{od}} = \langle p|H|h\rangle + \langle pp|H|hh\rangle + \boxed{\langle v|H|q\rangle + \langle pq|H|vv\rangle + \langle pp|H|hv\rangle}$$

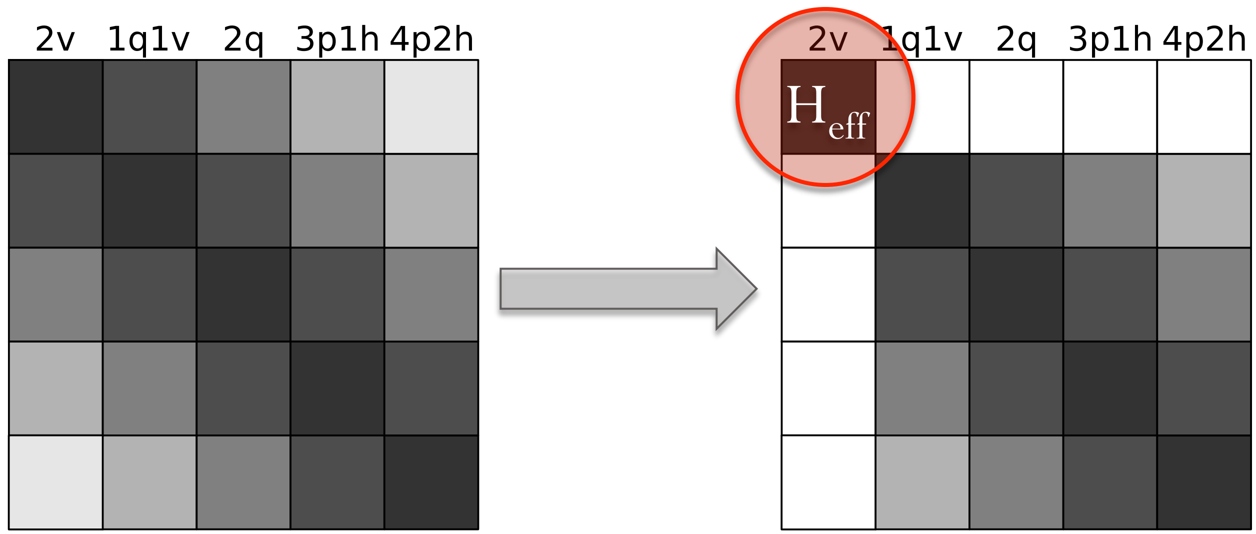
# IM-SRG: Valence-Space Formulation

**Open shell systems** Tsukiyama, Bogner, Schwenk, PRC (2012)

Split particle states into valence states, *v*, and those above valence space, *q*

Redefine "off-diagonal" to exclude valence particles




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

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

Inherently nonperturbative – no need for extended valence space?

# Nonperturbative Valence-Space Strategy

1) NN and 3N forces from Chiral EFT

2) Evolve with free-space SRG $\lambda_{SRG} = 1.88 - 2.24\text{fm}^{-1}$

3) Normal-order wrt HF reference state

4) Perform IM-SRG(2) calculation in flow-equation approach

5) Diagonalize with standard shell-model machinery

**NN matrix elements**

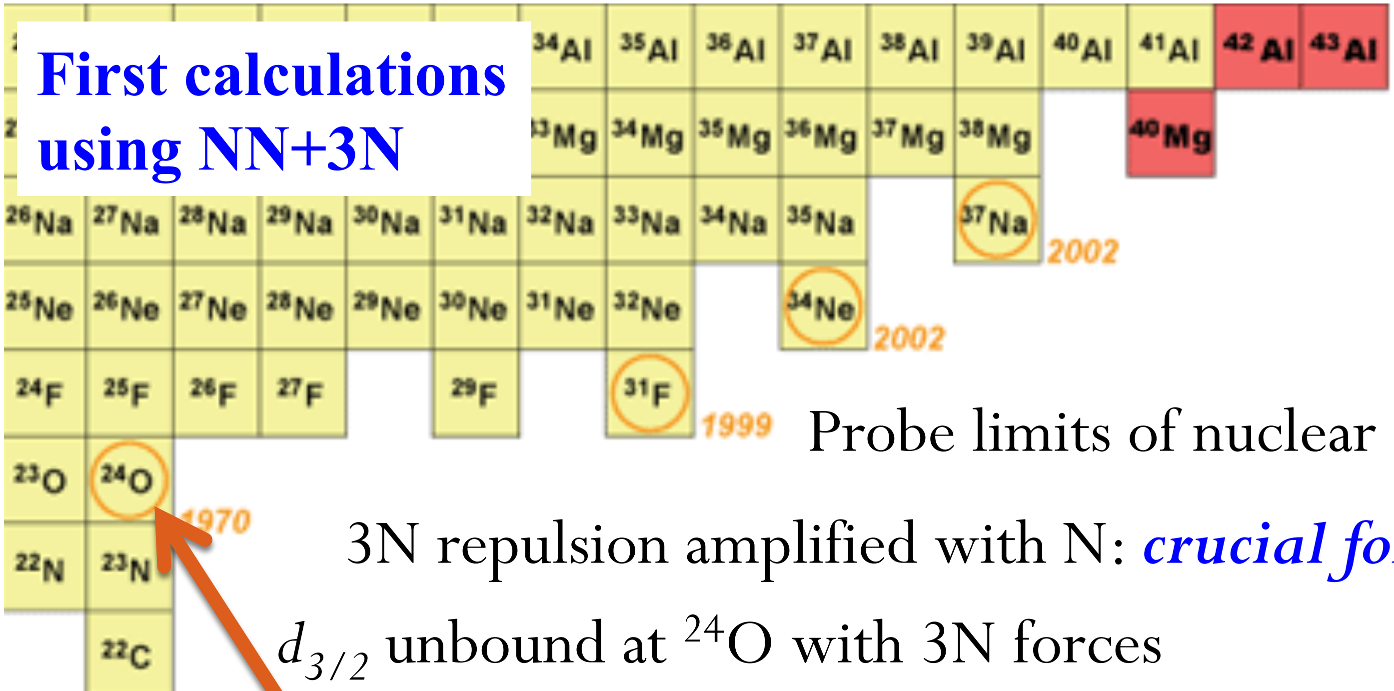
- $e_{max} = 2n + l = 14$ **converged**
- Vary $\hbar\omega = 20 - 24\text{MeV}$
- Consistently include 3N forces **induced** by SRG evolution (**NN+3N-ind**)

**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

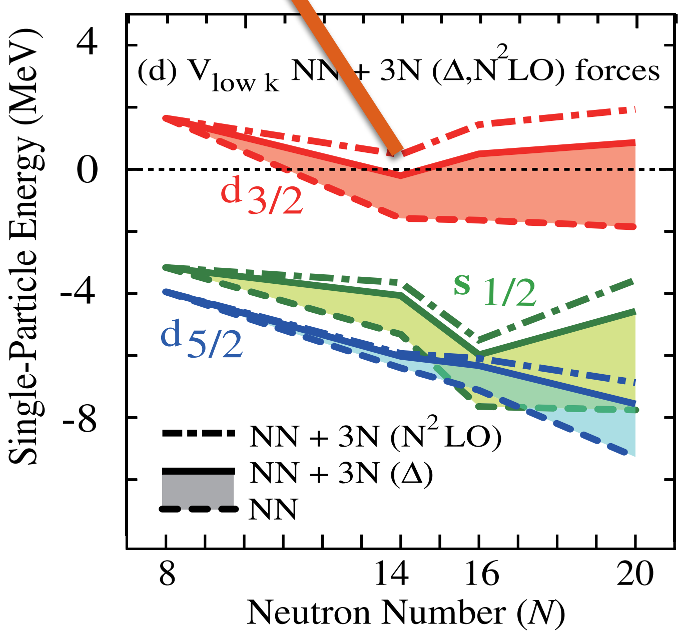
**First calculations using NN+3N**

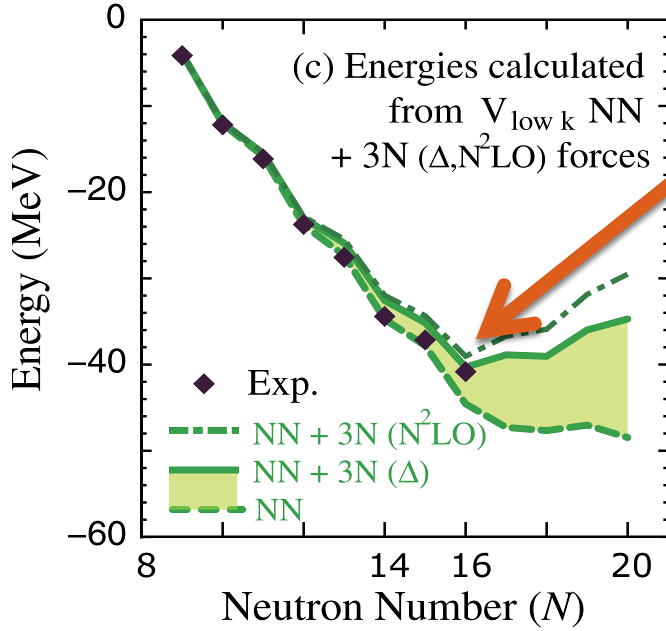



Probe limits of nuclear existence with 3N forces

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

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



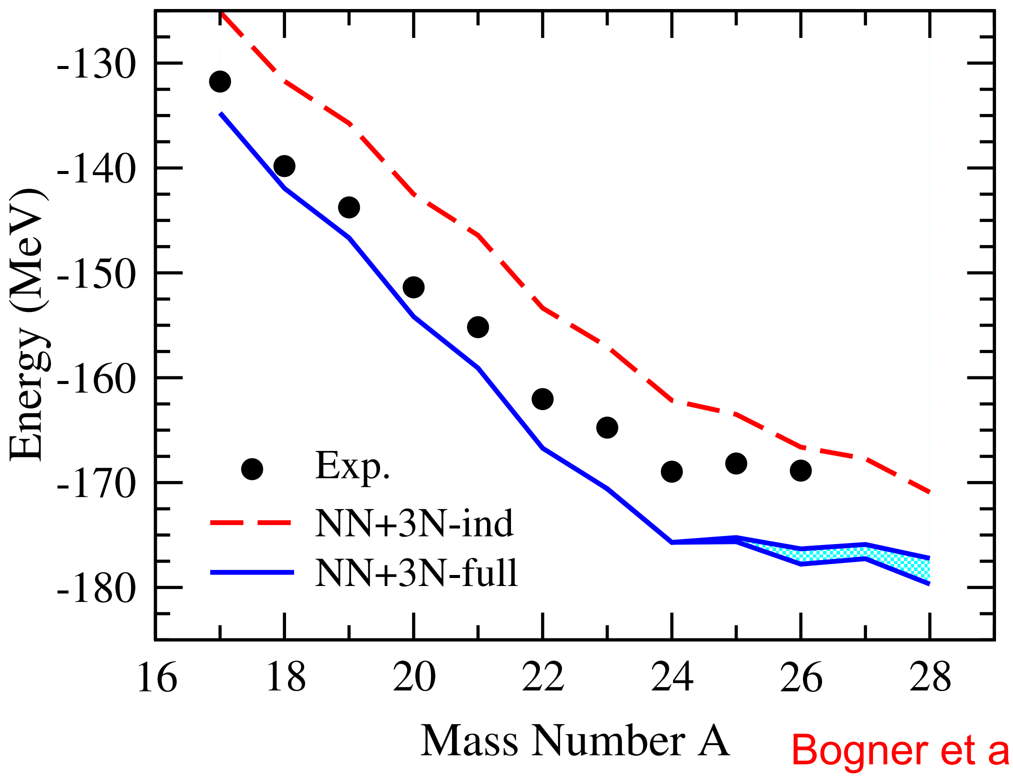

Isotopes unbound beyond $^{24}$O

**First microscopic explanation of oxygen anomaly**

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

# IM-SRG Oxygen Ground-State Energies

Valence-space interaction and SPEs from IM-SRG in *sd* shell




Bogner et al., PRL (2014)

NN+3N-induced reproduce exp well, not dripline

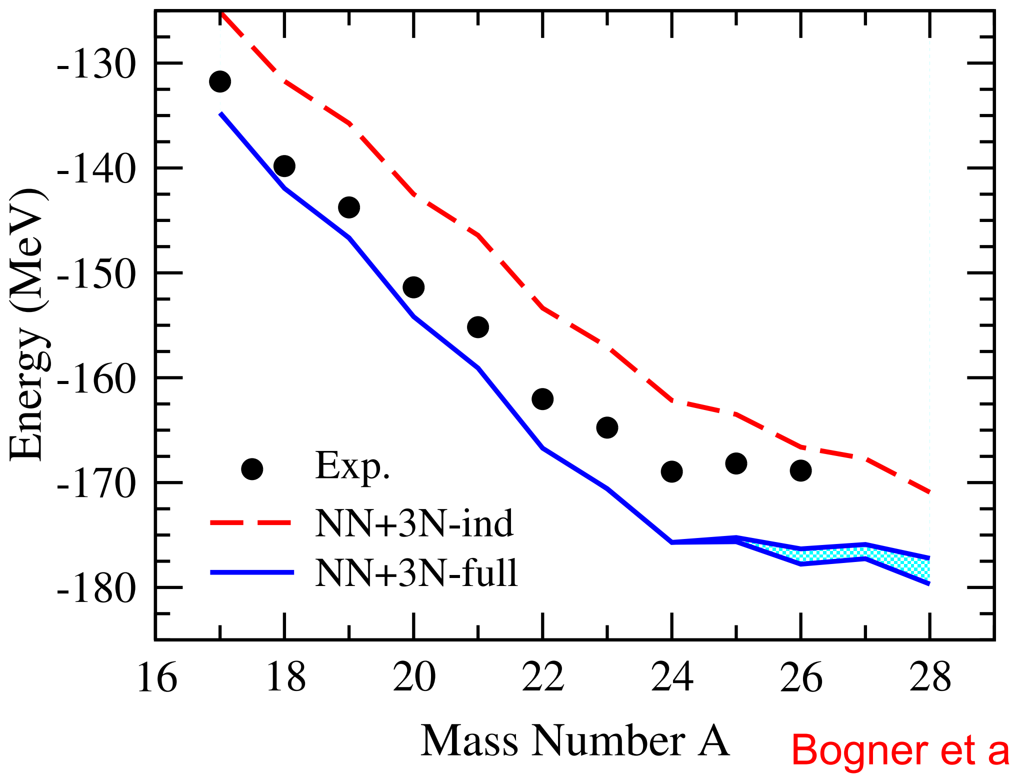
NN+3N-full modestly overbound – good behavior past dripline

Good dripline properties

Very weak $\hbar\omega$ dependence

# Comparison with Large-Space Methods

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

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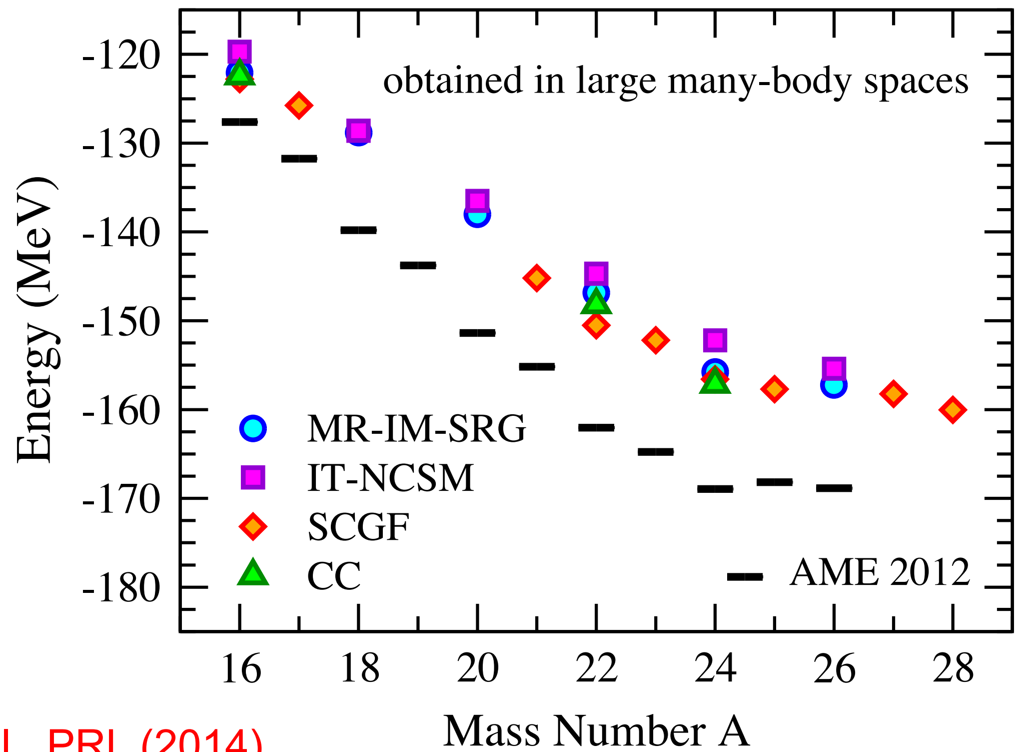


Clear improvement with full NN+3N

Validates valence-space results

Remarkable agreement between all methods with same forces

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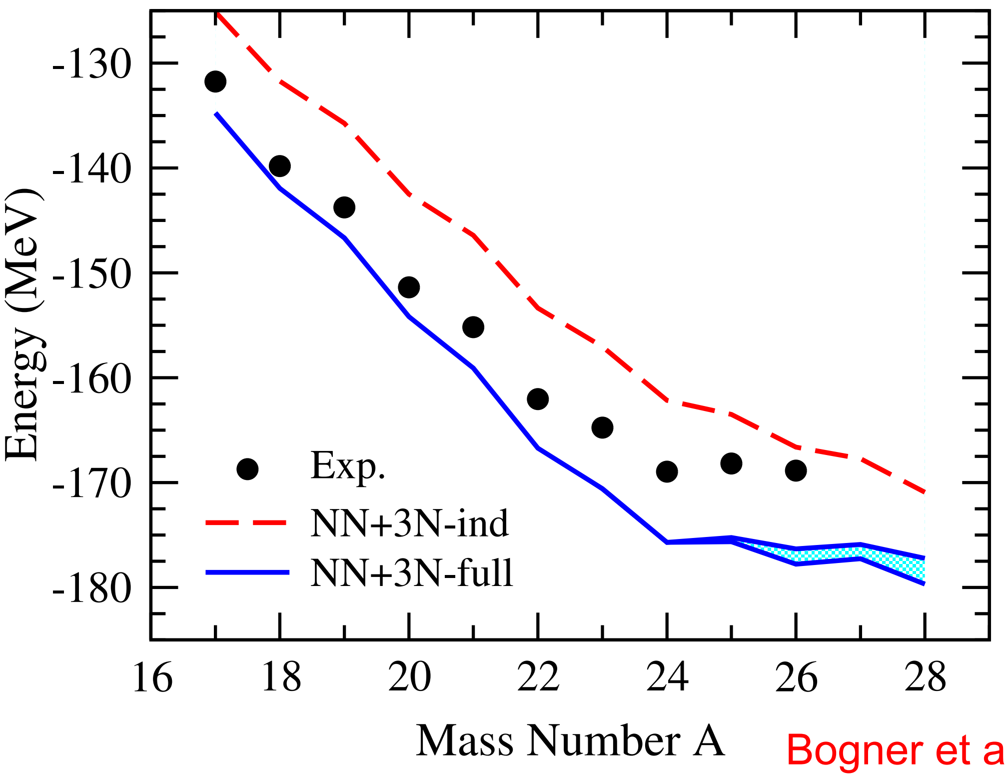


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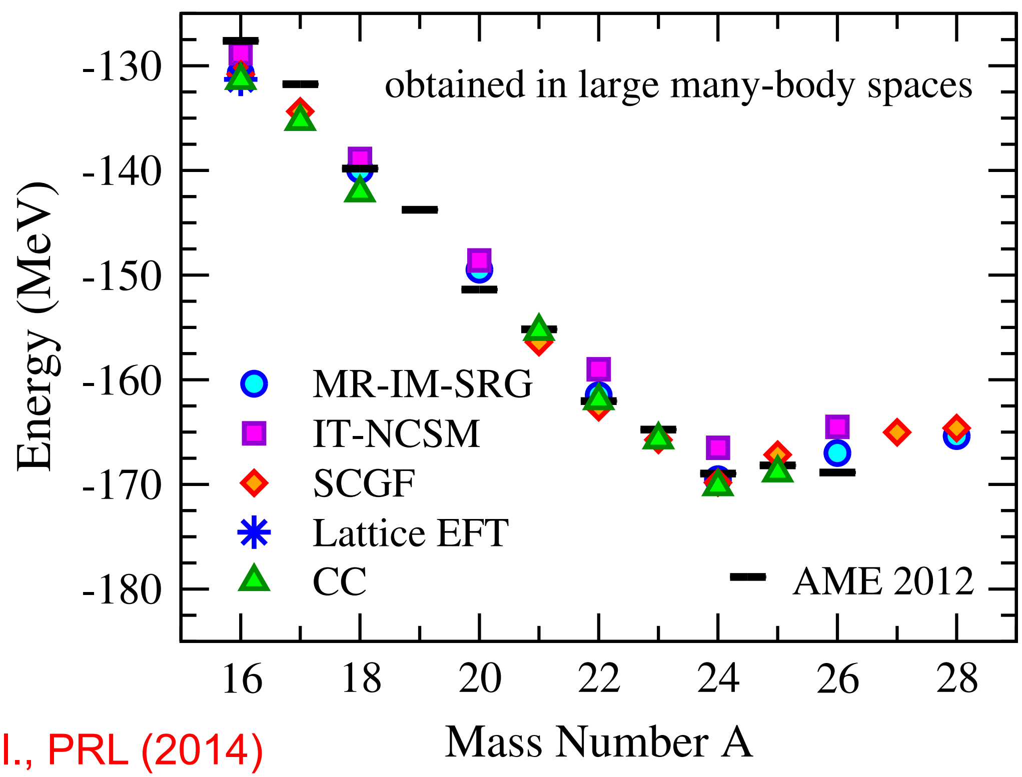


Hebeler, JDH, Menéndez, Schwenk, ARNPS (2015)

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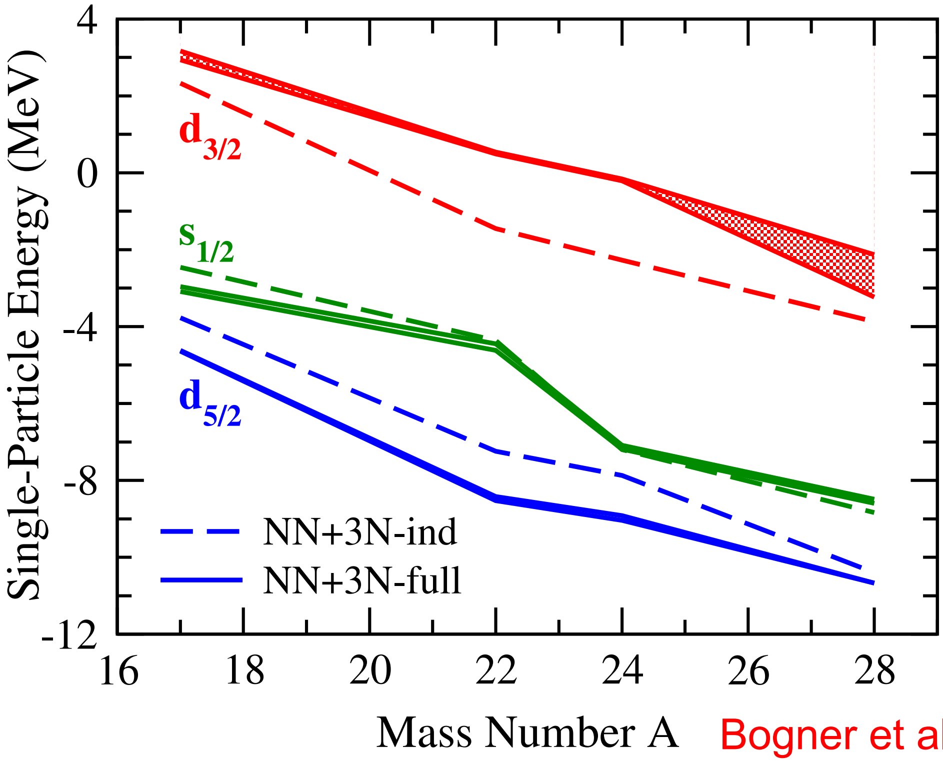
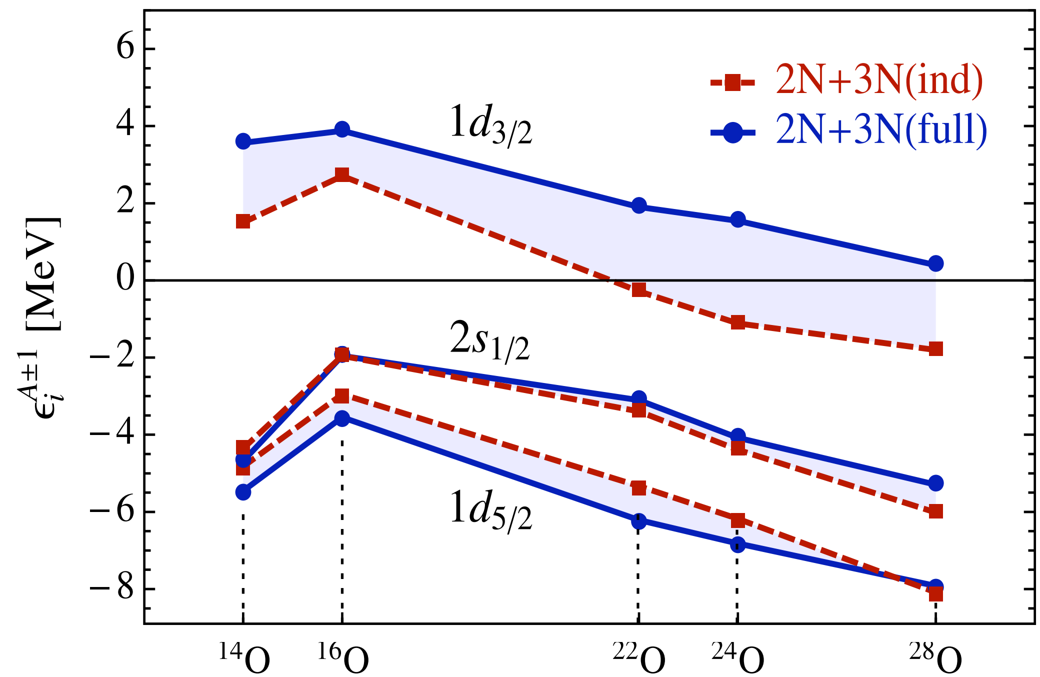
# Dripline Mechanism

Compare to large-space methods with same SRG-evolved NN+3N forces




Bogner et al., PRL (2014)




Cipollone, Barbieri, Navrátil, PRL (2013)

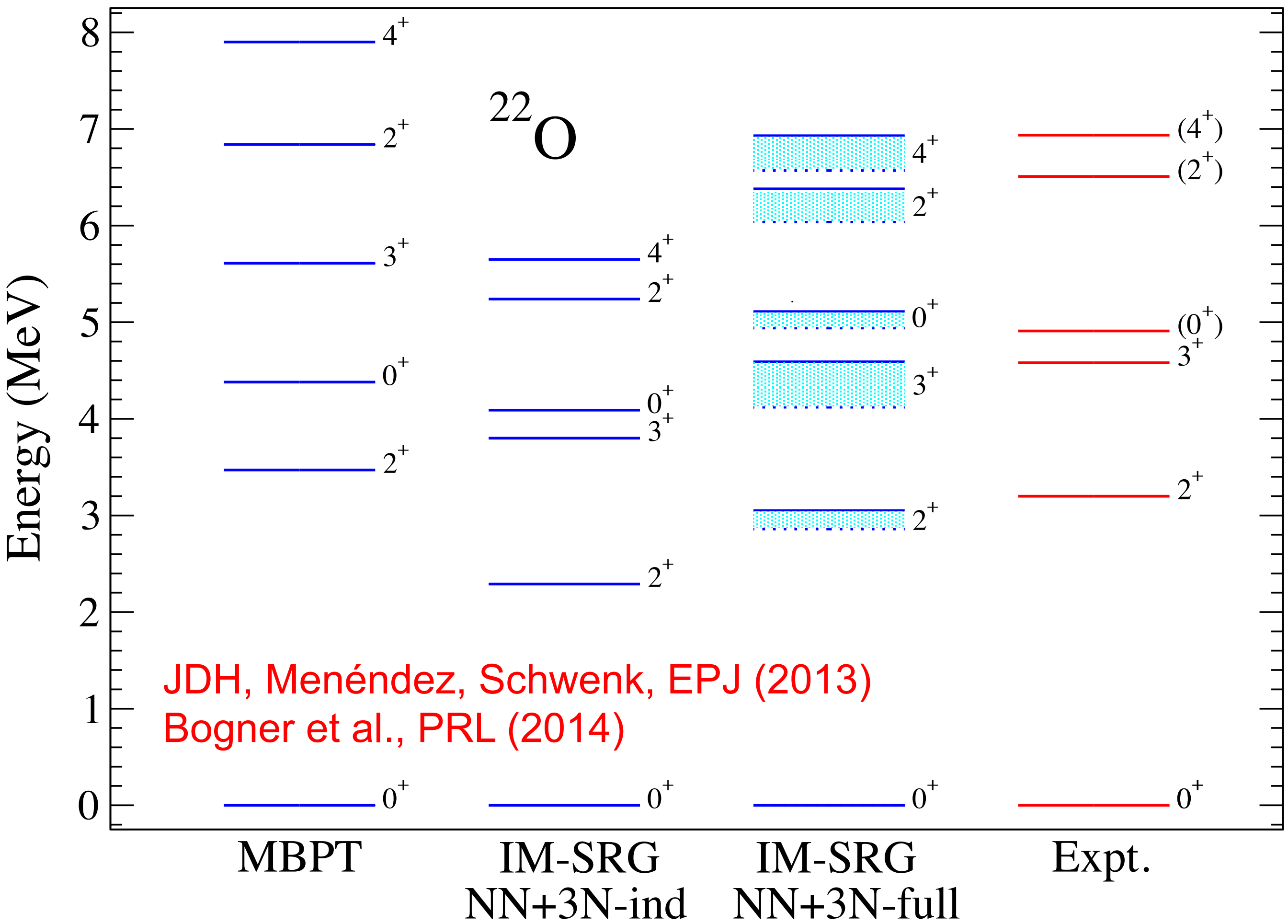
Robust mechanism driving dripline behavior

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 IM-SRG




Clear improvement with NN+3N-full

IM-SRG: comparable with phenomenology

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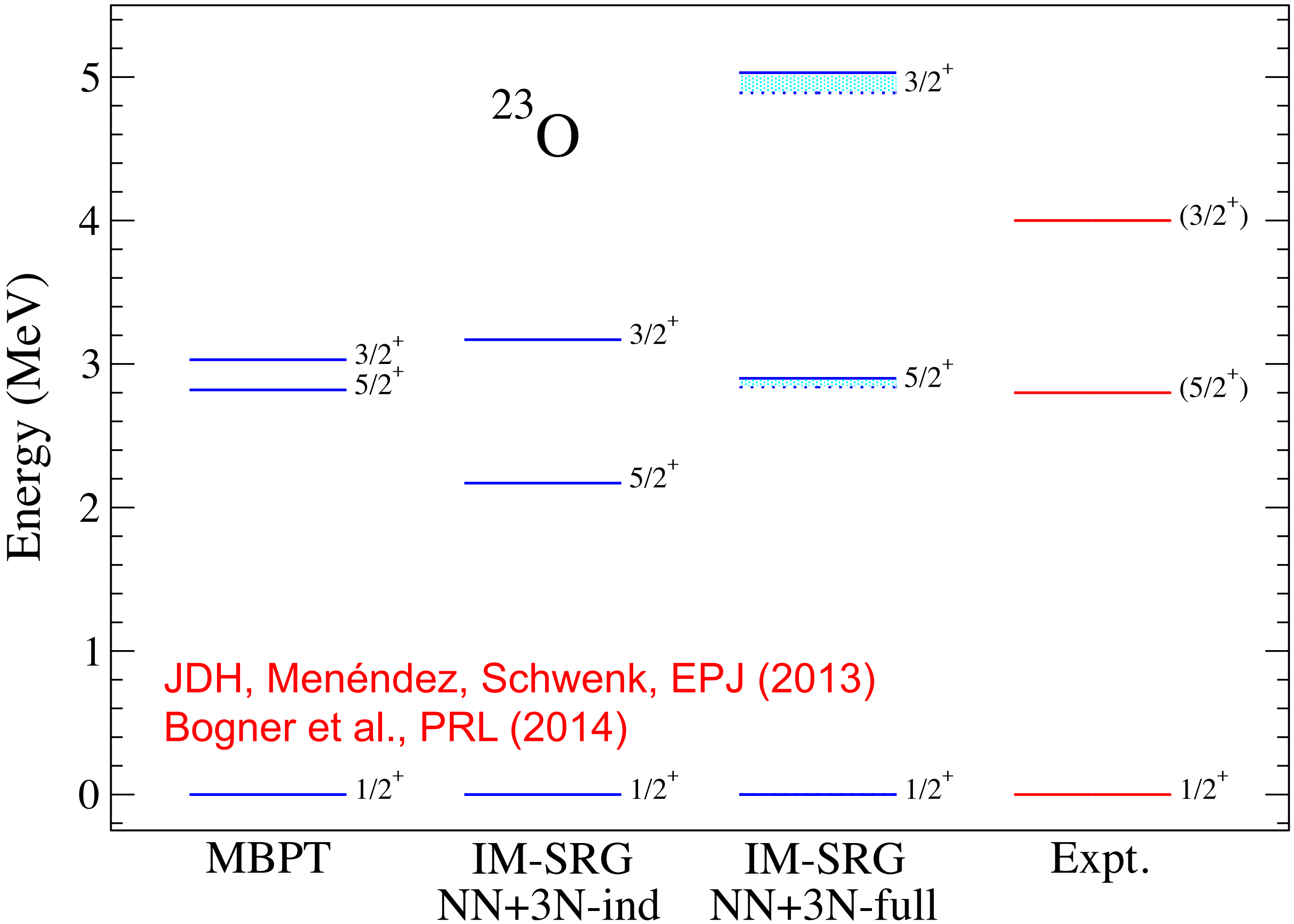
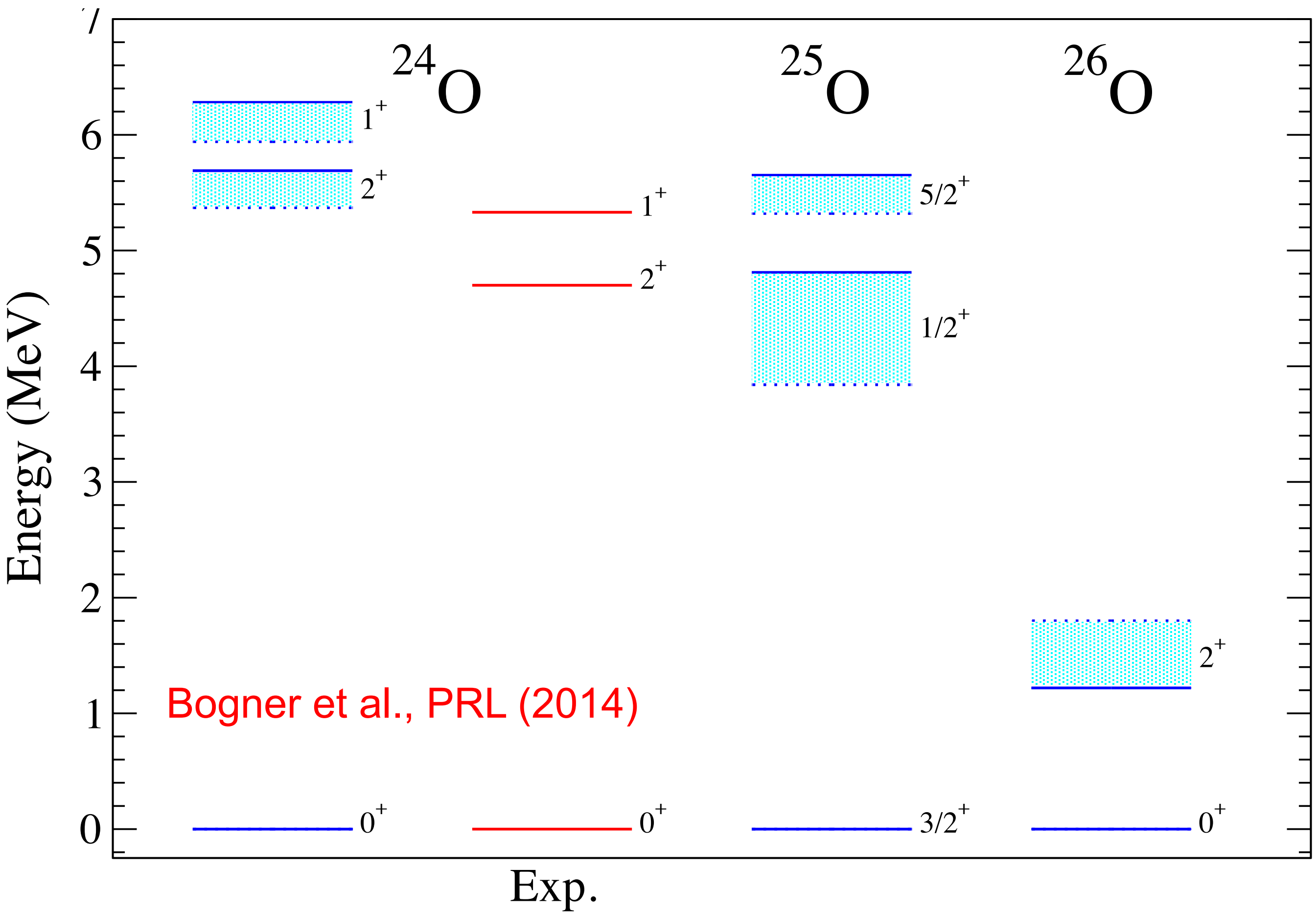



Clear improvement with NN+3N-full

Continuum neglected: expect to lower $d_{3/2}$

# IM-SRG Oxygen Spectra

Oxygen spectra: IM-SRG predictions beyond the dripline



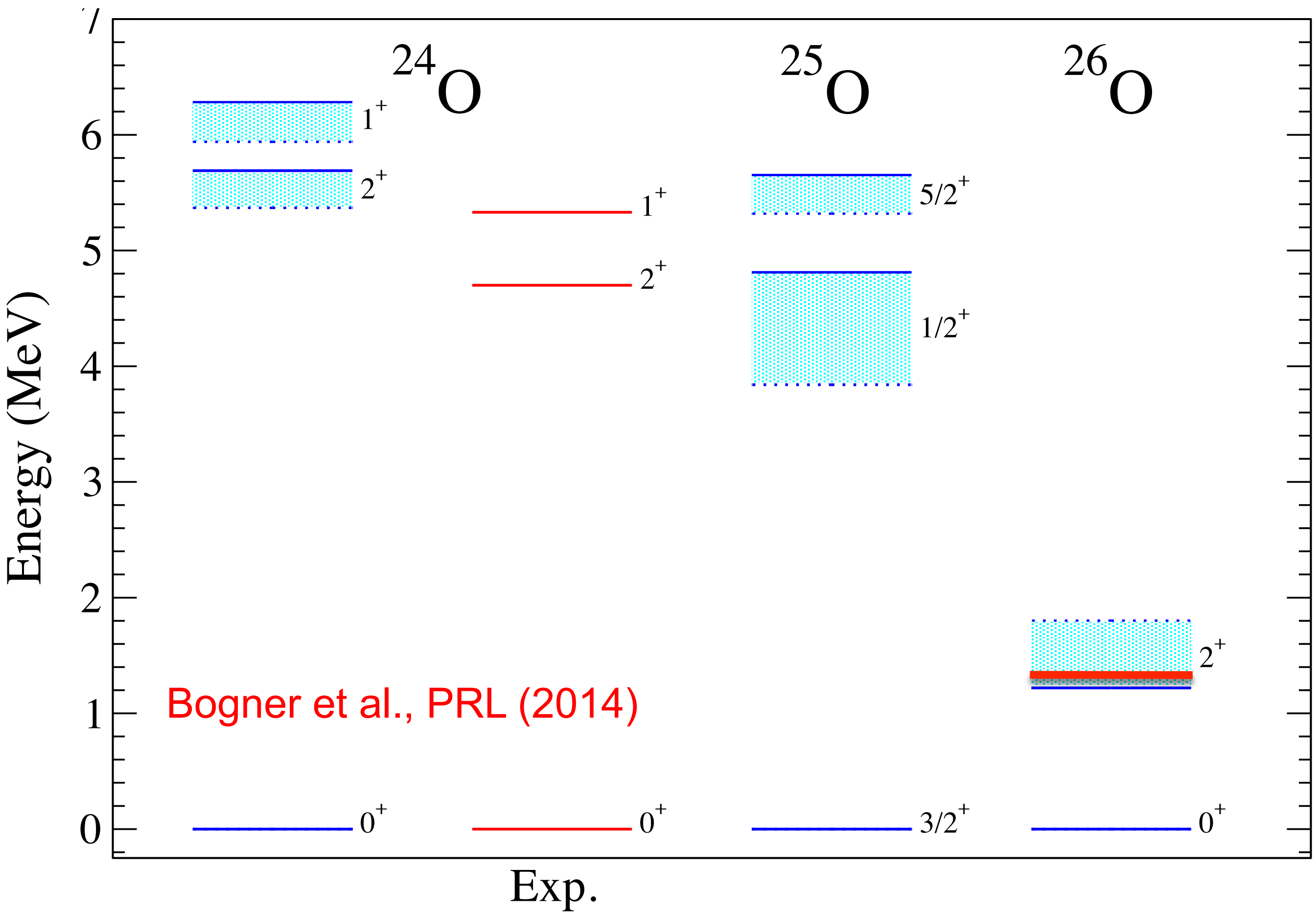

$^{24}$O closed shell (too high $2^+$)

Continuum neglected: expect to lower spectrum

Only one excited state in $^{26}$O below 6.5MeV

# Experimental Connection: $^{26}$O Spectrum

Oxygen spectra: IM-SRG predictions beyond the dripline




Kondo et al., PRELIMINARY

New measurement at RIKEN on excited states in $^{26}$O

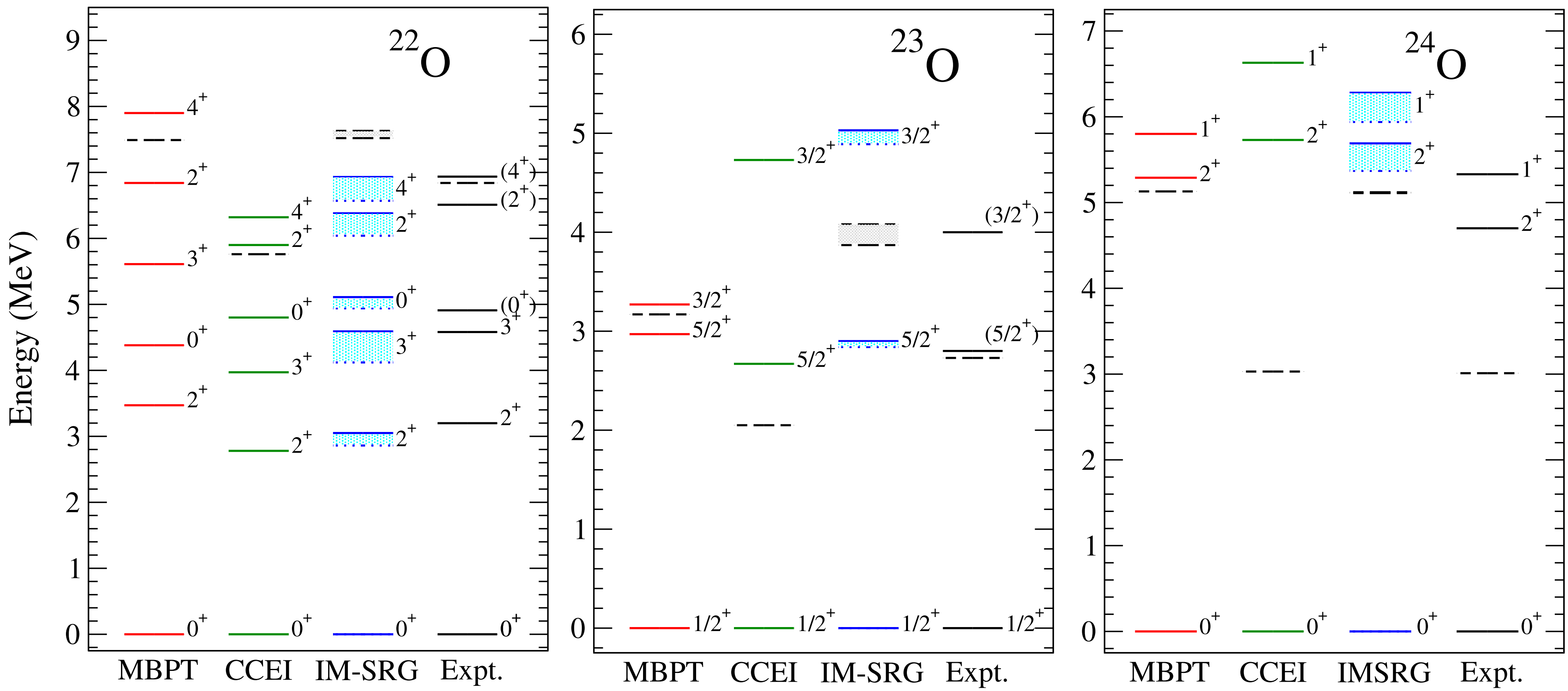
Existence of excited state 1.3MeV

**IM-SRG prediction: one natural-parity state below 7MeV at 1.22MeV**

# Comparison with MBPT/CCEI Oxygen Spectra

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

See talk of **G. Hagen**



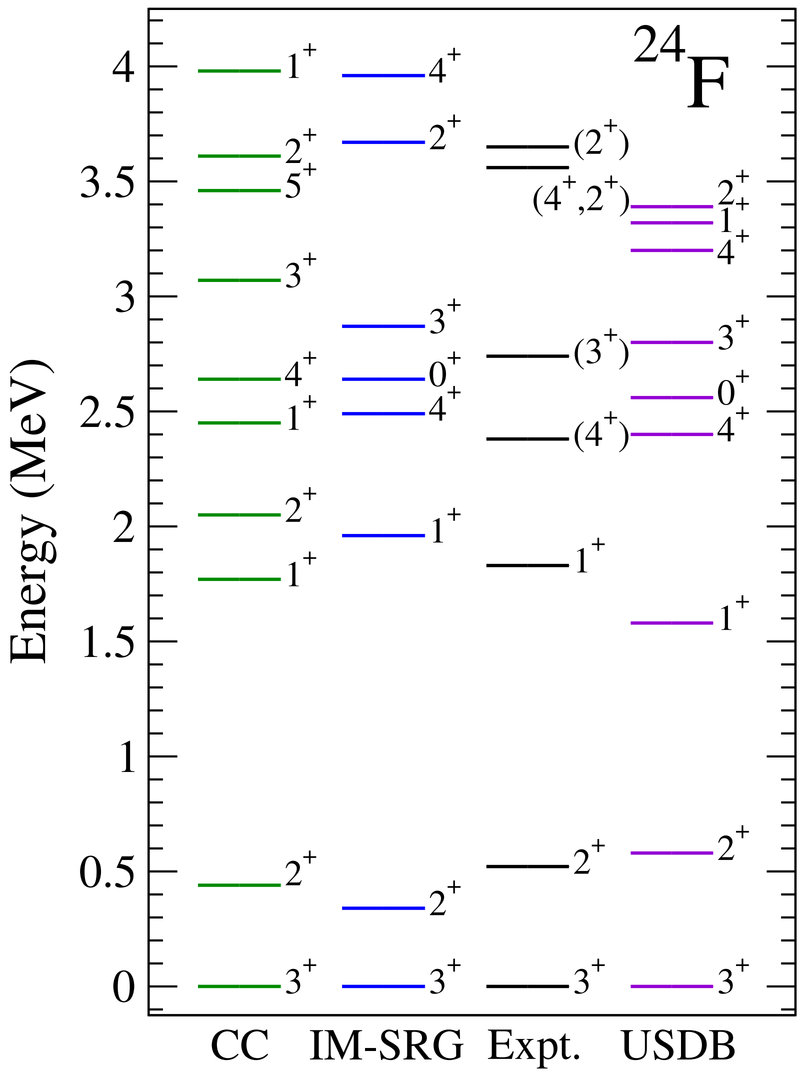

Hebeler, JDH, Menéndez, Schwenk, ARNPS (2015)

**MBPT** in extended valence space

IM-SRG/CCEI spectra agree within ~300 keV

# Experimental Connection: $^{24}$F Spectrum

$^{24}$F spectrum: extended-space MBPT and (sd-shell) IM-SRG, full CC




Ekström et al., PRL (2014)

Cáceres et al., arXiv:1501.01166

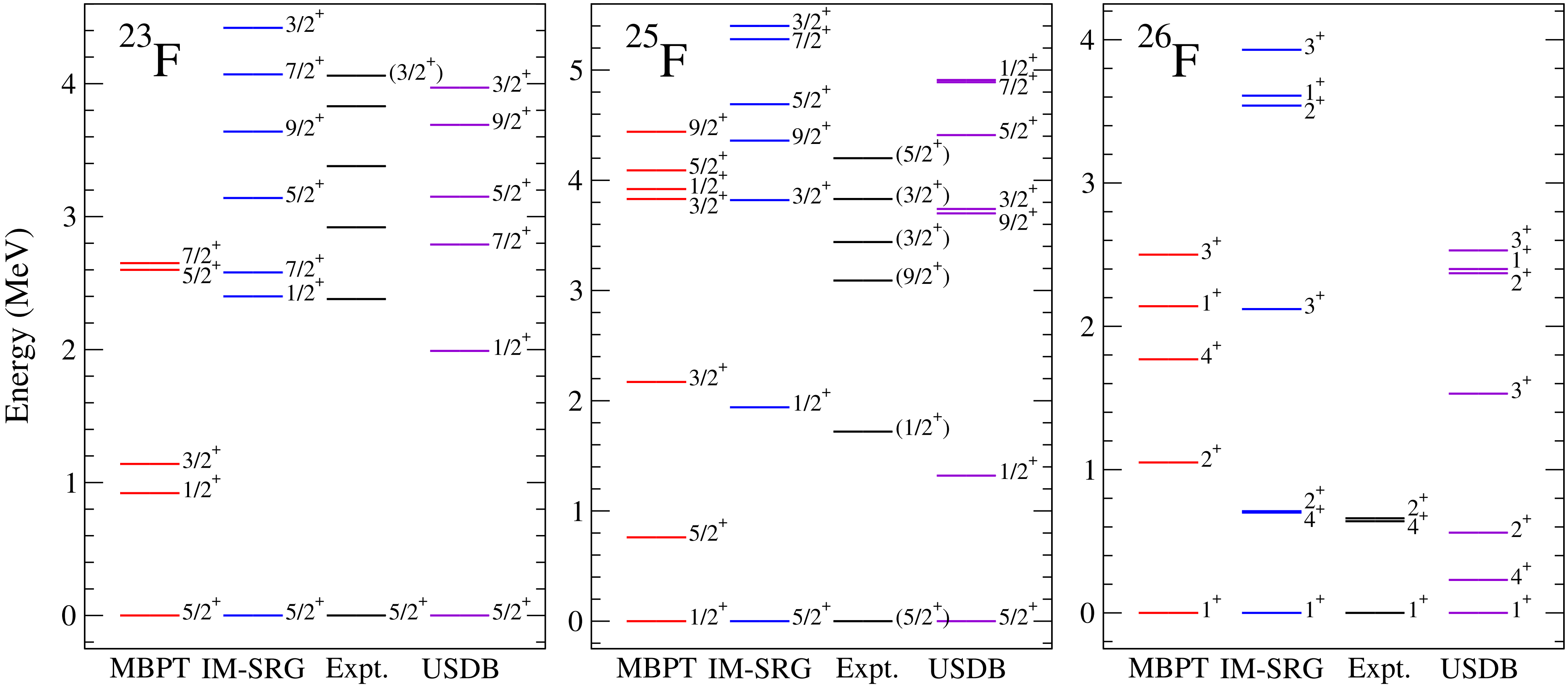
Hebeler, JDH, Menéndez, Schwenk, ARNPS (2015)

**New measurements from GANIL**

IM-SRG: comparable with phenomenology in good agreement with new data

# Fully Open Shell: Neutron-Rich Fluorine Spectra

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



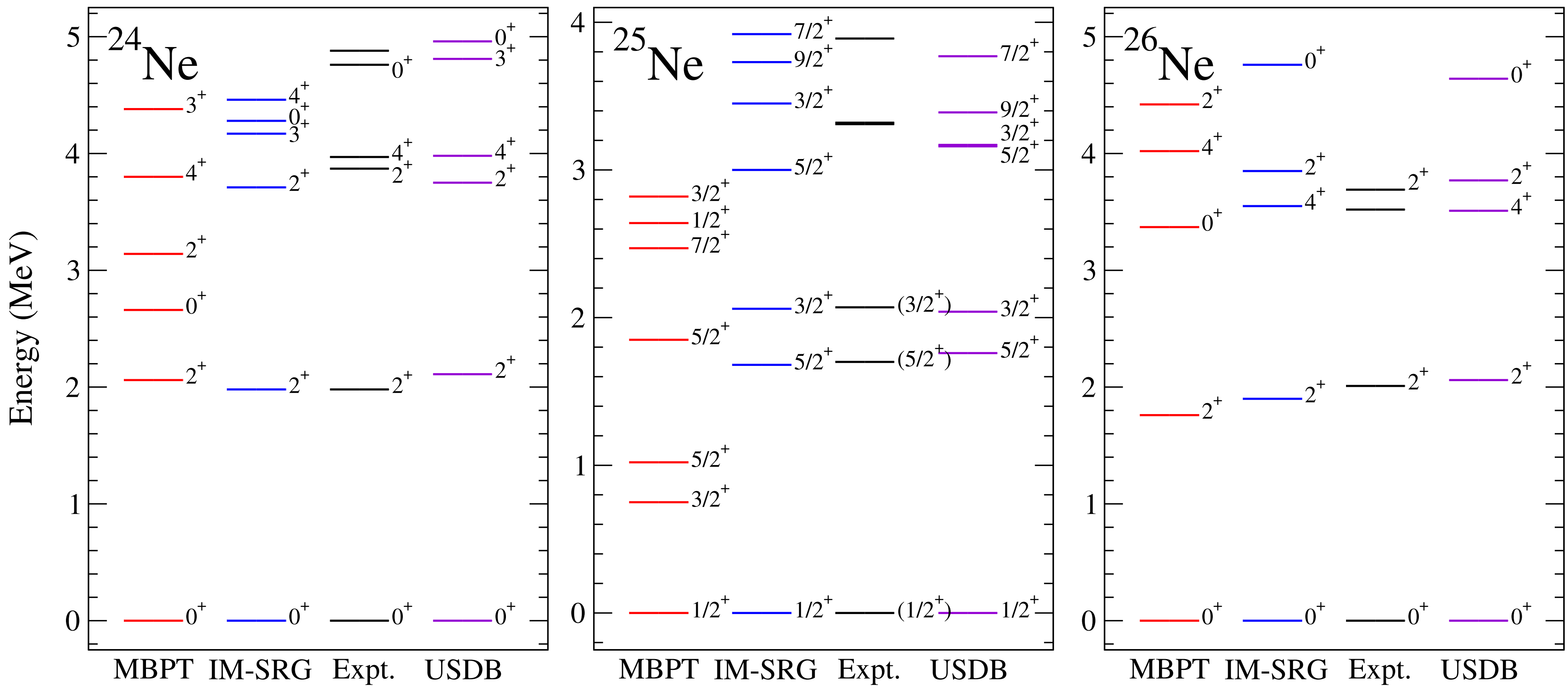

Bogner, Hergert, JDH, Schwenk, in prep.

MBPT: obvious deficiencies

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

# Fully Open Shell: Neutron-Rich Neon Spectra

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




Bogner, Hergert, JDH, Schwenk, in prep.

MBPT: obvious deficiencies

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

# Alternative Approach: Magnus Expansion

**Magnus expansion:** explicitly construct unitary transformation *U(s)*

$$U(s) = e^{\Omega(s)}$$

With flow equation:

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

Leads to commutator expression for evolved Hamiltonian

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

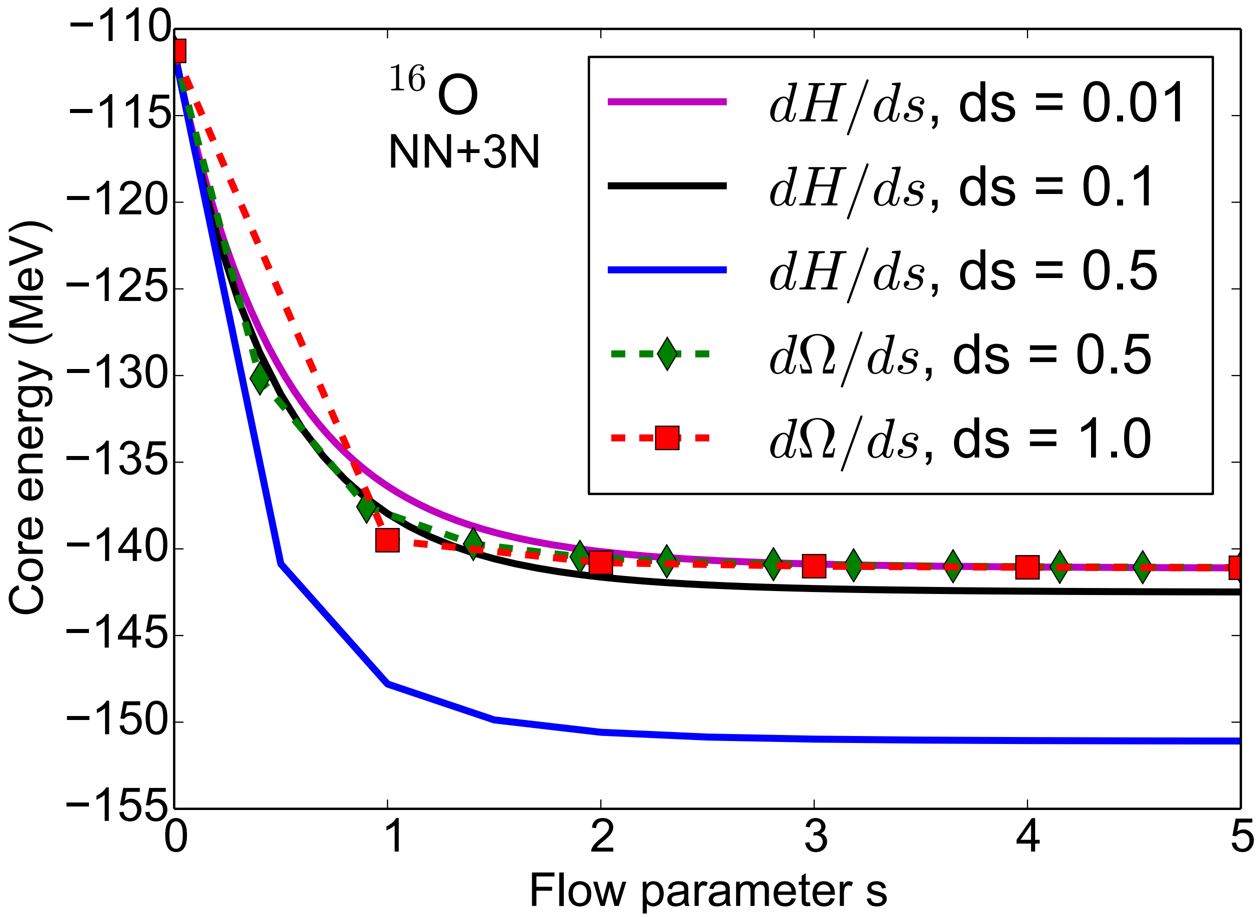
**Morris**, **Parzuchowski**, Bogner, in prep

Nested commutator series – in practice truncate numerically

**Perform all calculations at two-body level**

# Magnus vs Flow-Equation

Analogous to electron gas results varying step size

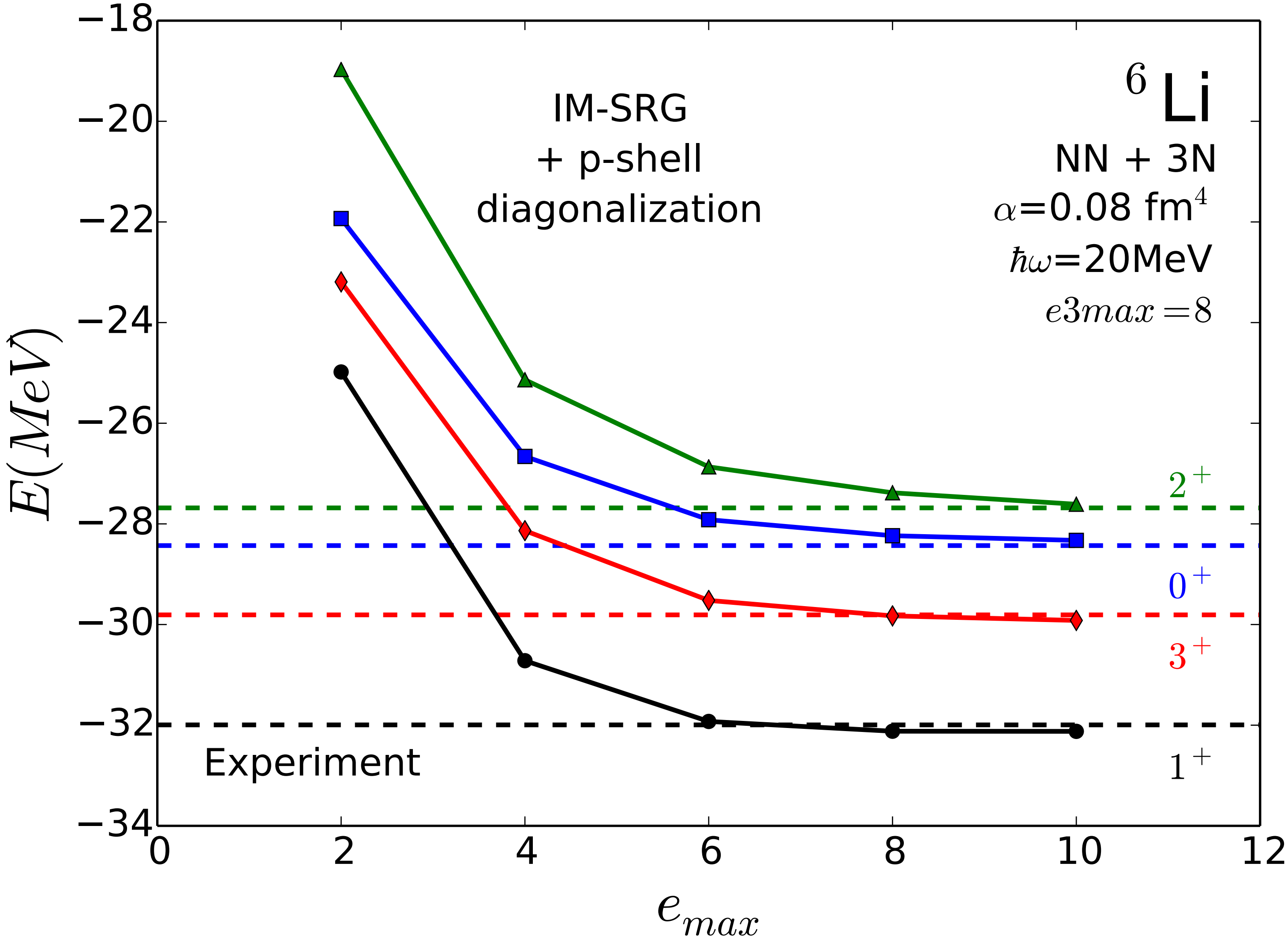



**Evident error accumulation in flow-equation for small step sizes**

**Magnus: rapid convergence, independent of step size**

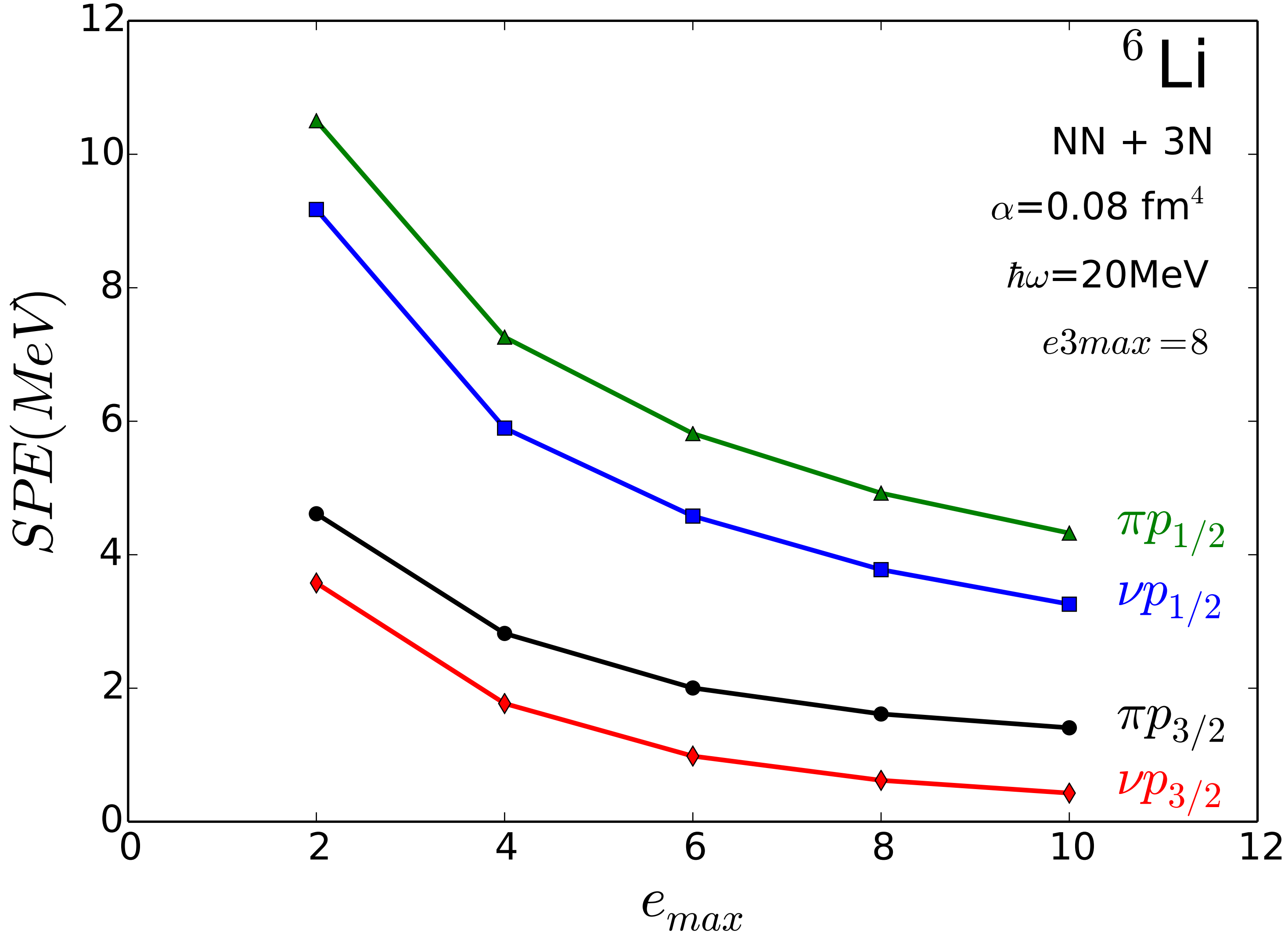
# p-Shell Benchmarks

## $^6$Li spectrum from NN+3N forces



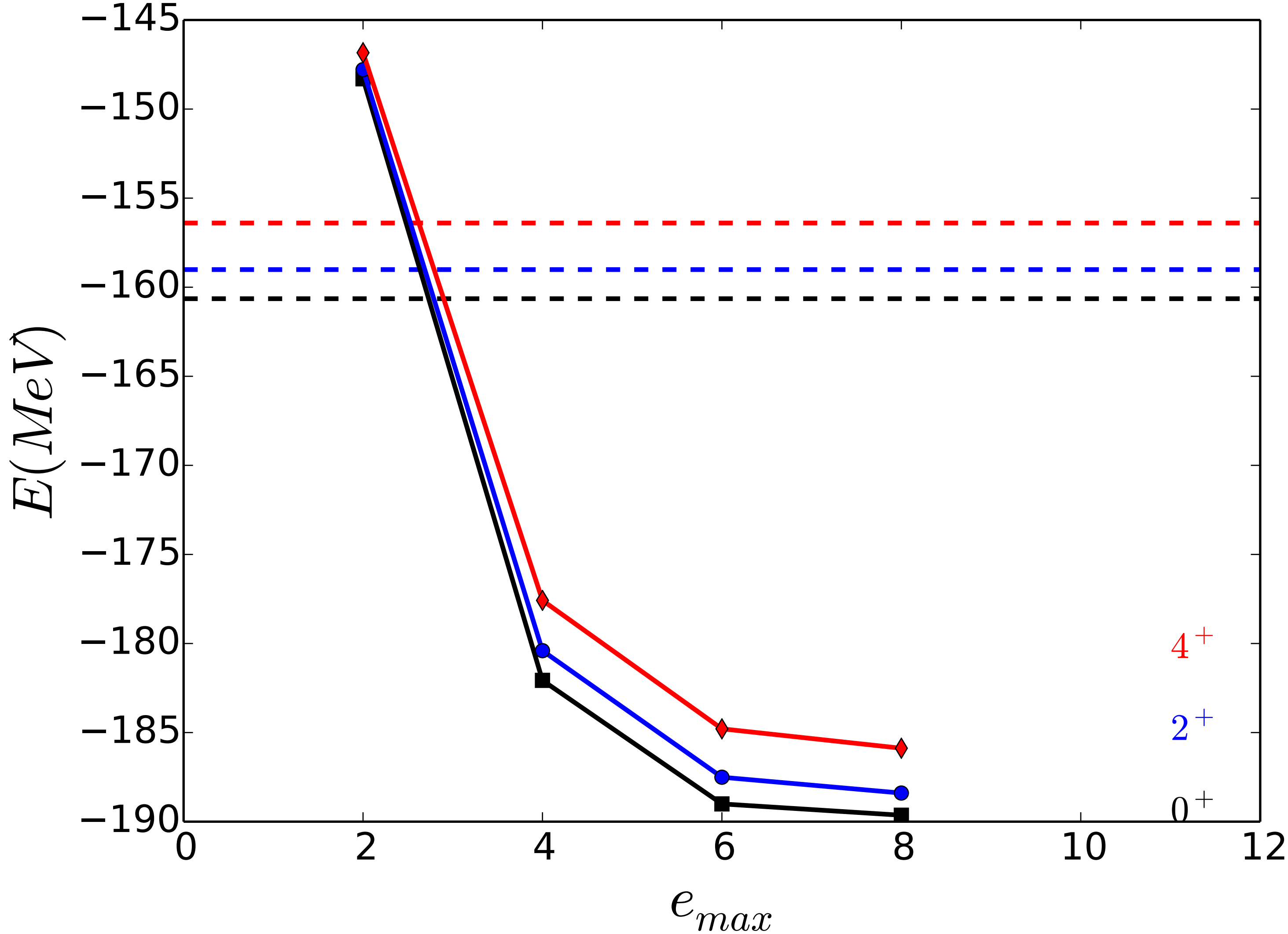
# p-Shell Benchmarks

## p-shell SPEs nearly converged



# sd-Shell Benchmarks

**$^{20}$Ne shell energies nearly converged**




**As in oxygen, overbound but spectrum well reproduced**

# Effective Operators

## Keep unitary transformation from evolution of Hamiltonian

Can generalize to arbitrary operators

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

$$\Downarrow$$

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

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

First apply to scalar operators

# E0 Transitions

Seldom calculated in nuclear shell model

**In single HO shell:**

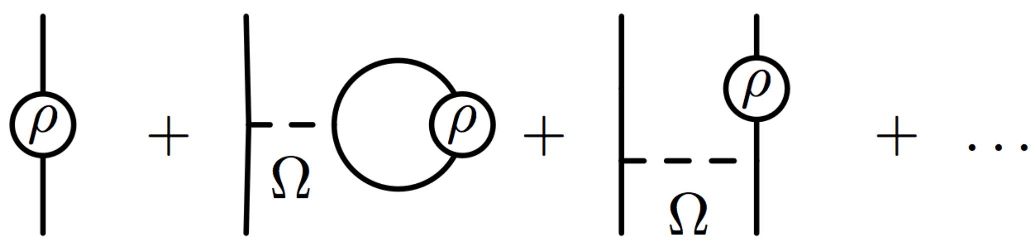
$$\left|\langle f|\rho_{E0}|i\rangle\right|^2 \propto \delta_{fi}; \quad \rho_{E0} = \frac{1}{e^2 R}\sum_i e_i r_i^2$$

Must resort to phenomenological gymnastics

With **Magnus IM-SRG**, calculate effective valence-space operator:

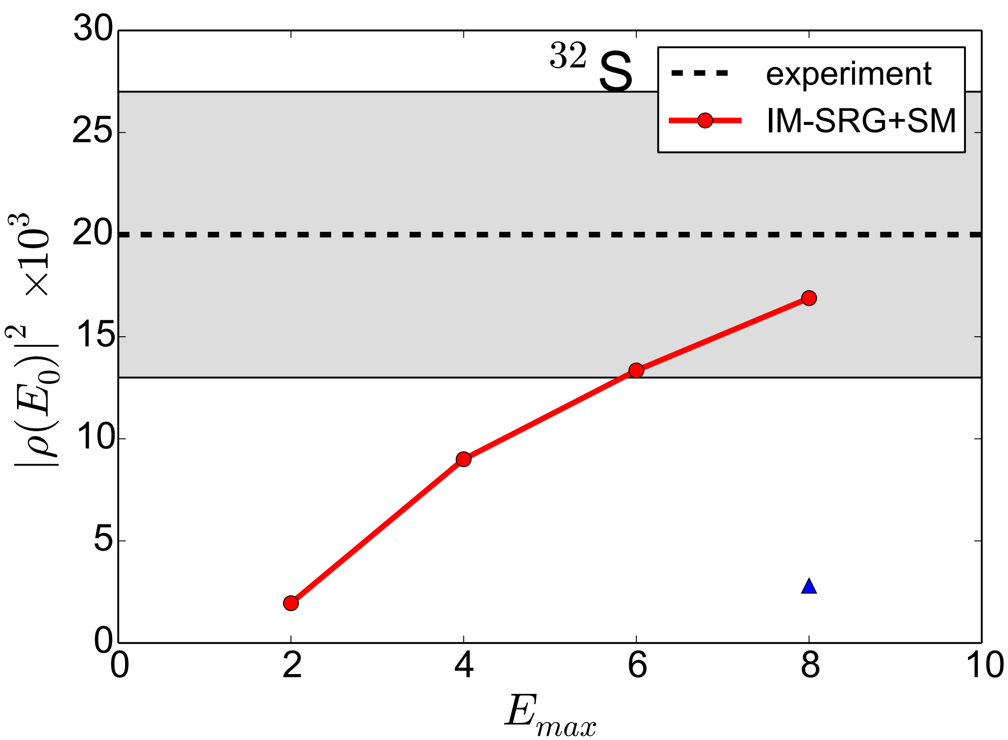
$$\rho_{E0}(s) = e^{\Omega(s)}\rho_{E0}e^{-\Omega(s)} = \rho_{E0} + \frac{1}{2}\left[\Omega(s),\rho_{E0}\right] + \cdots$$

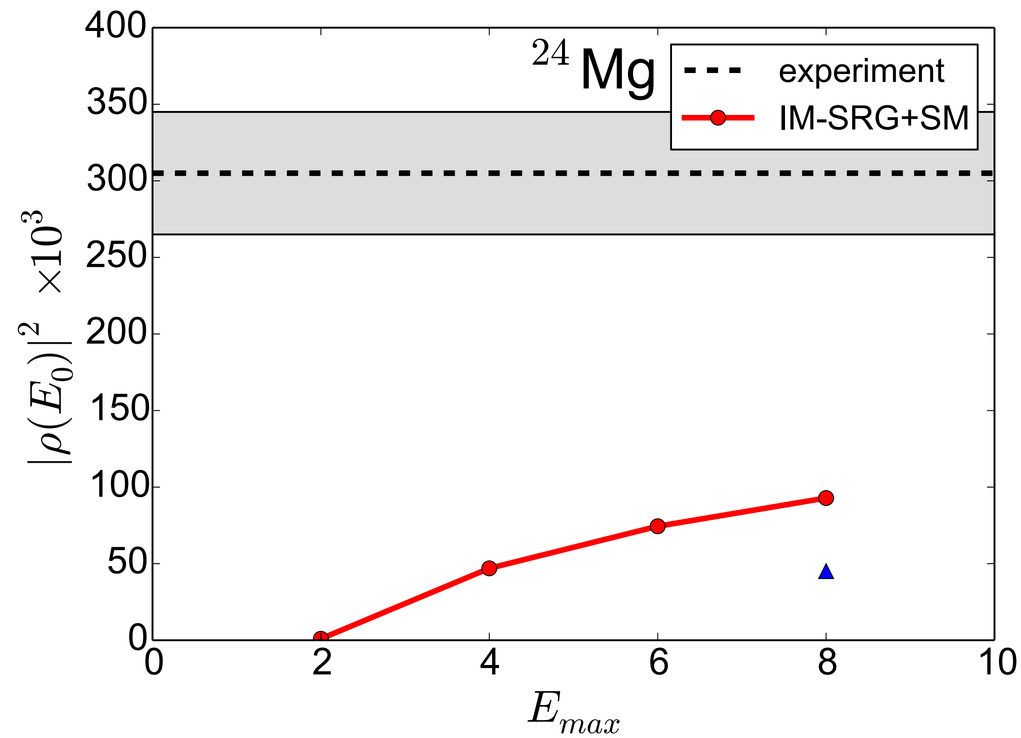
**Commutators induce important two-body parts**



# E0 Transitions in sd Shell Model

**Very preliminary** results in *sd* shell (not converted in NN or 3N):



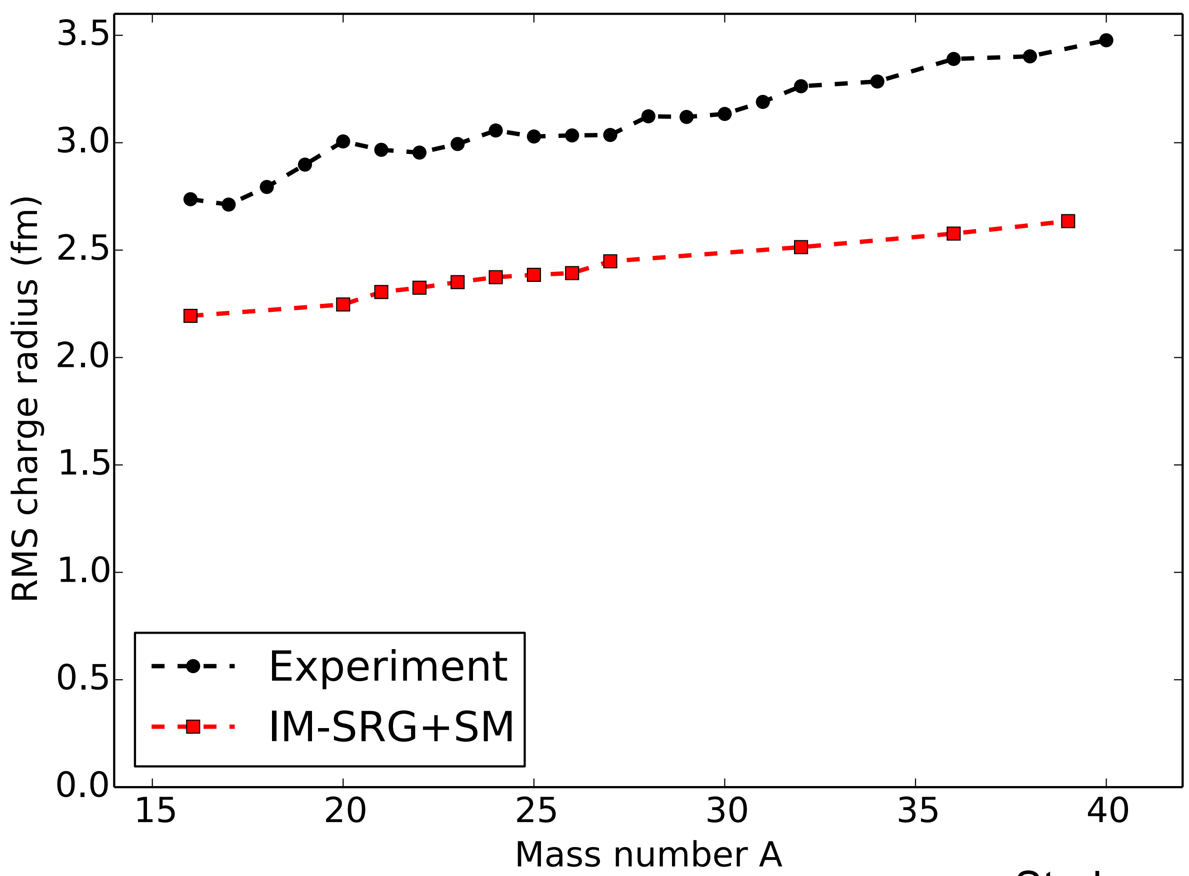

**3N forces provide significant reduction**

**Need additional benchmarks**

# RMS Charge Radii in sd Shell Model

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

**Radii for stable sd-shell nuclei calculated in shell model NN+3N**




Stroberg et al, in prep

# 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

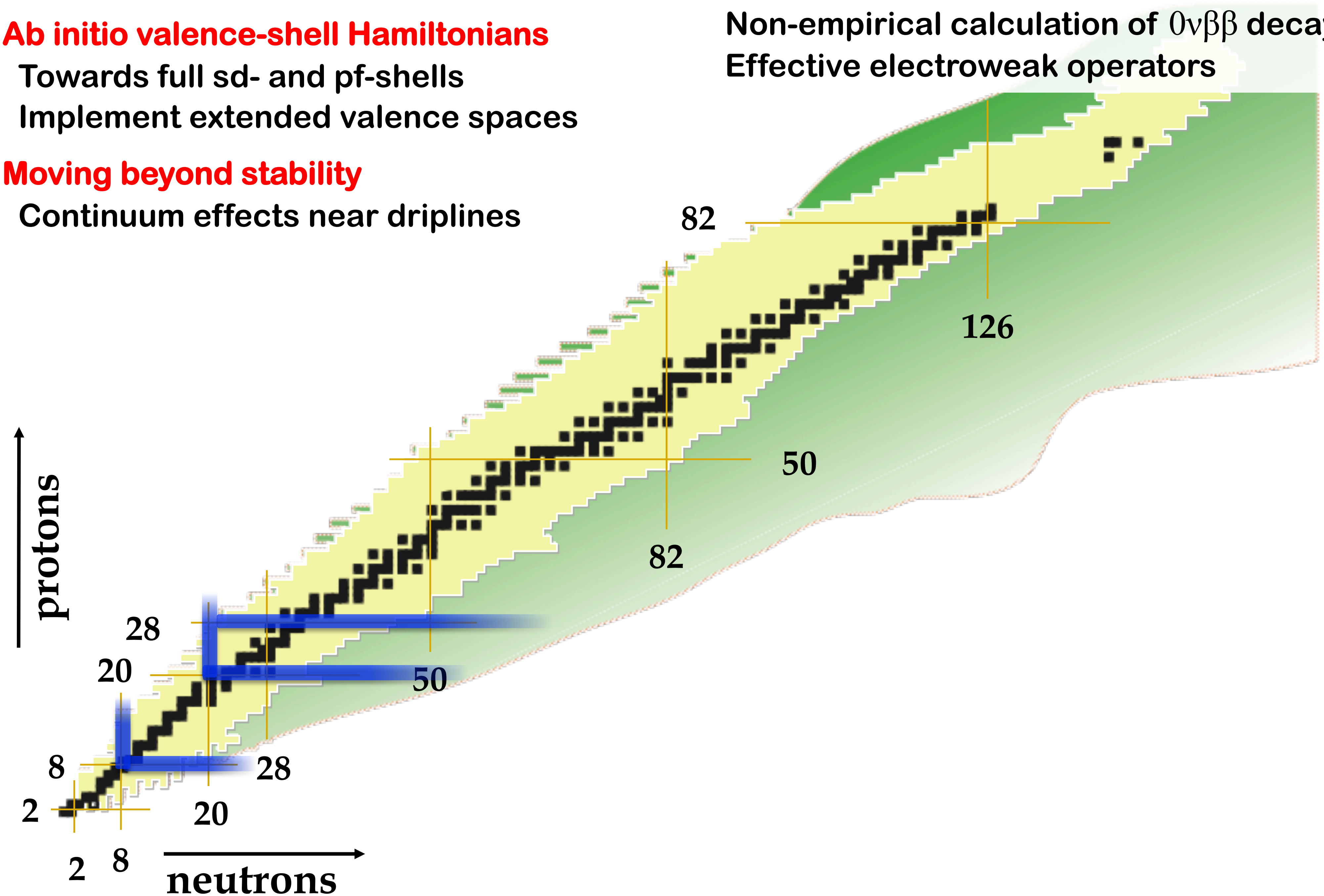
**Moving beyond stability**

Continuum effects near driplines

**Fundamental symmetries**

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

Effective electroweak operators



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- Implement extended valence spaces

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- Effective electroweak operators