Towards Ab Initio Calculations of Double-Beta Decay Nuclear Matrix Elements

Jason D. Holt

NRC·CNRC

TRIUMF

NSERC
CRSNG

JÜLICH
FORSCHUNGSZENTRUM

TRIUMF **R. Stroberg**

TECHNISCHE
UNIVERSITÄT
DARMSTADT **A. Schwenk**

MICHIGAN STATE
UNIVERSITY **S. Bogner** **H. Hergert**

THE UNIVERSITY
of NORTH CAROLINA
at CHAPEL HILL **J. Engel**

CMU
CENTRAL MICHIGAN
UNIVERSITY **M. Horoi**

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

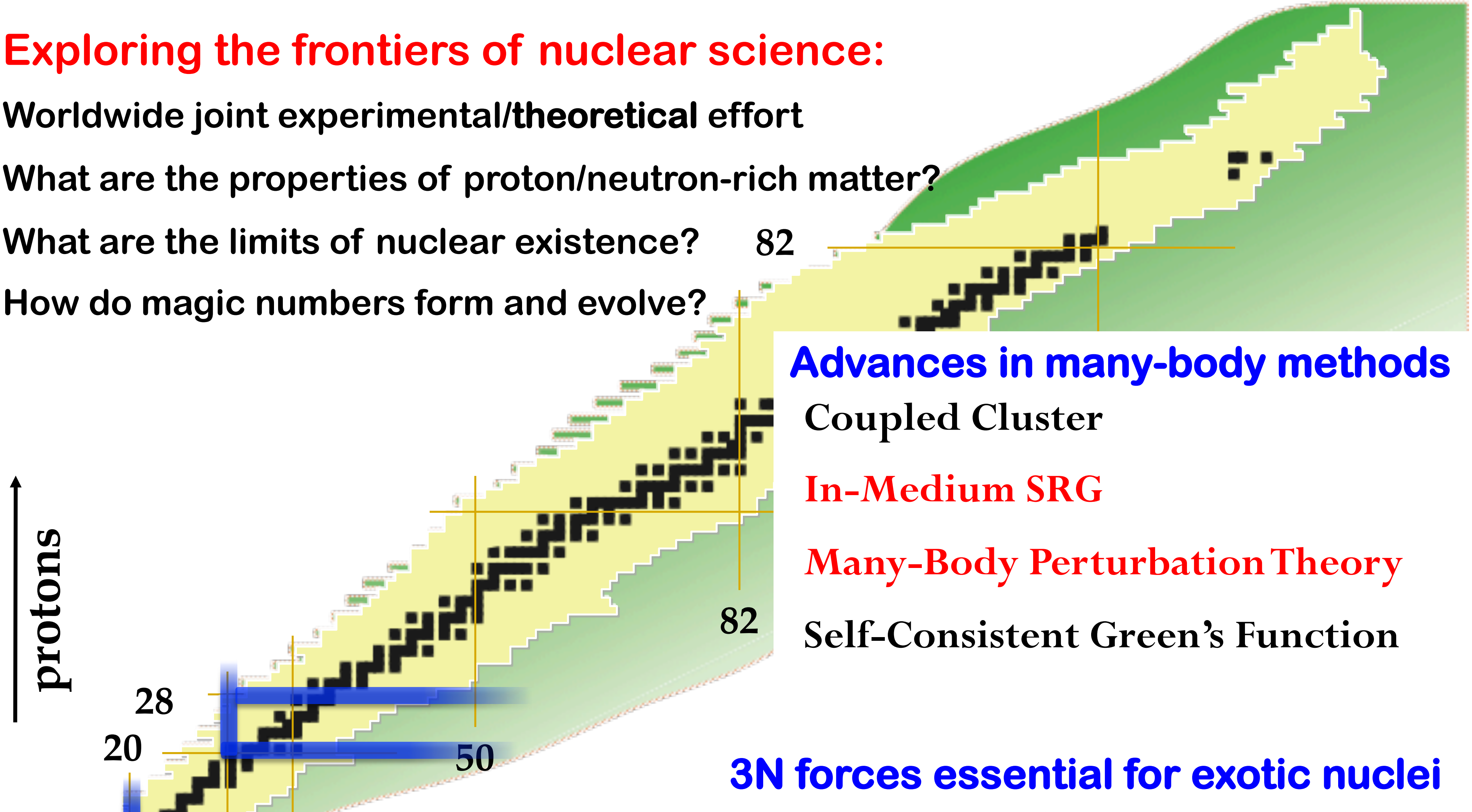
Exploring the frontiers of nuclear science:

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?



Advances in many-body methods

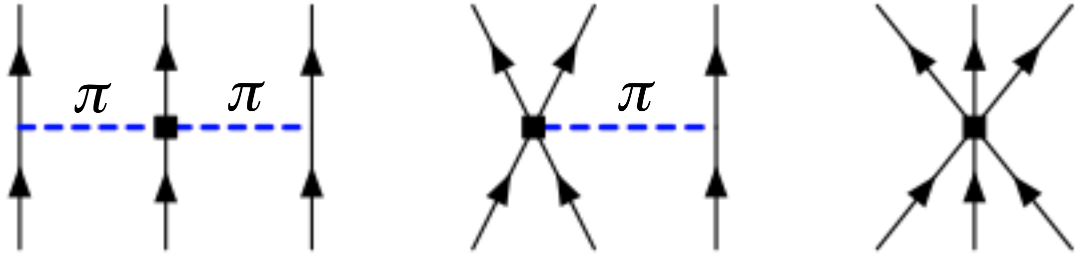
Coupled Cluster

In-Medium SRG

Many-Body Perturbation Theory

Self-Consistent Green’s Function

3N forces essential for exotic nuclei



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

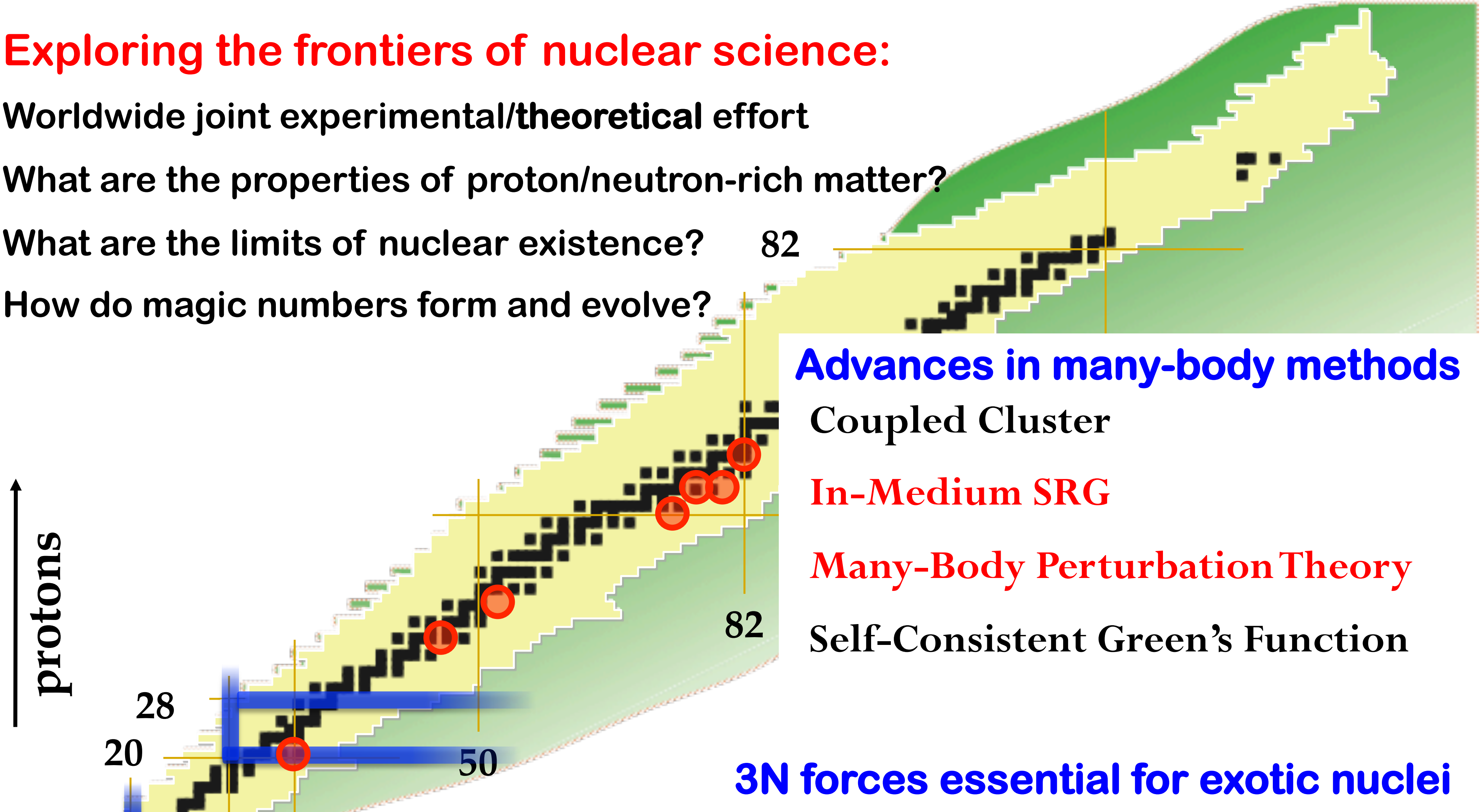
Exploring the frontiers of nuclear science:

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?



Advances in many-body methods

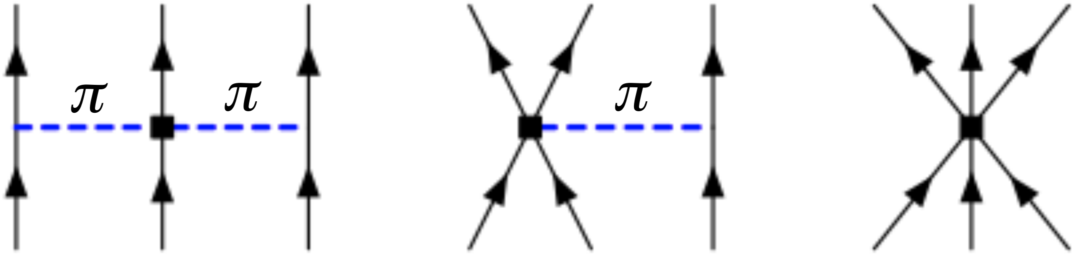
Coupled Cluster

In-Medium SRG

Many-Body Perturbation Theory

Self-Consistent Green's Function

3N forces essential for exotic nuclei



Improved 0νββ-Decay Calculations in Shell Model

Standard SM approach: phenomenological wavefunctions + **bare** operator

Avenue towards ab initio shell-model calculations:

Consistent operators and wfs from chiral forces and currents

$$M^{0\nu} = M^{0\nu}_{GT} - \frac{M^{0\nu}_F}{g_A^2} + M^{0\nu}_T$$

$$M^{0\nu}_{GT} = \langle f | \sum_{ab} H(r_{ab}) \sigma_a \cdot \sigma_b \; \tau_a^+ \tau_b^+ | i \rangle$$

1) **Wavefunctions** currently phenomenological; **calculate ab initio**

IM-SRG, CC, MBPT… Part II

Improved 0νββ-Decay Calculations in Shell Model

Standard SM approach: phenomenological wavefunctions + **bare** operator

Avenue towards ab initio shell-model calculations:

Consistent operators and wfs from chiral forces and currents

$$M^{0\nu} = M^{0\nu}_{GT} - \frac{M^{0\nu}_{F}}{g_A^2} + M^{0\nu}_{T}$$

$$M^{0\nu}_{GT} = \langle f|\sum_{ab} H(r_{ab})\,\sigma_a\cdot\sigma_b\;\tau_a^+\tau_b^+|i\rangle$$

M_{eff}

1) Wavefunctions currently phenomenological; calculate ab initio
2) **Effective decay operator**: **correlations outside valence space**

MBPT… Part I

Improved 0νββ-Decay Calculations in Shell Model

Standard SM approach: phenomenological wavefunctions + **bare** operator

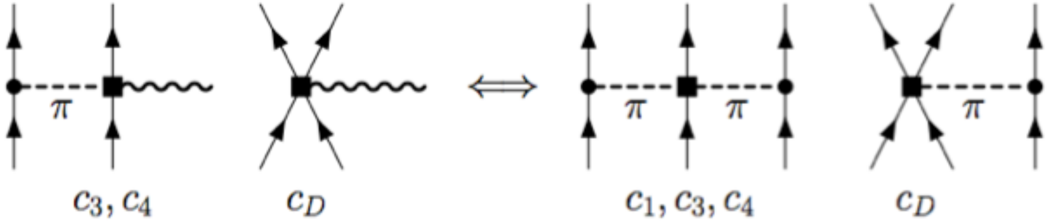
Avenue towards ab initio shell-model calculations:

Consistent operators and wfs from chiral forces and currents

$$M^{0\nu} = M^{0\nu}_{GT} - \frac{M^{0\nu}_{F}}{g_A^2} + M^{0\nu}_{T}$$

$$M^{0\nu}_{GT} = \langle f | \sum_{ab} H(r_{ab}) \sigma_a \cdot \sigma_b \; \tau_a^+ \tau_b^+ | i \rangle$$

1) Wavefunctions currently phenomenological; calculate ab initio
2) Effective decay operator: correlations outside valence space
3) Operator corrections: **two-body currents**



See talks of Menéndez, Gazit, Schwenk

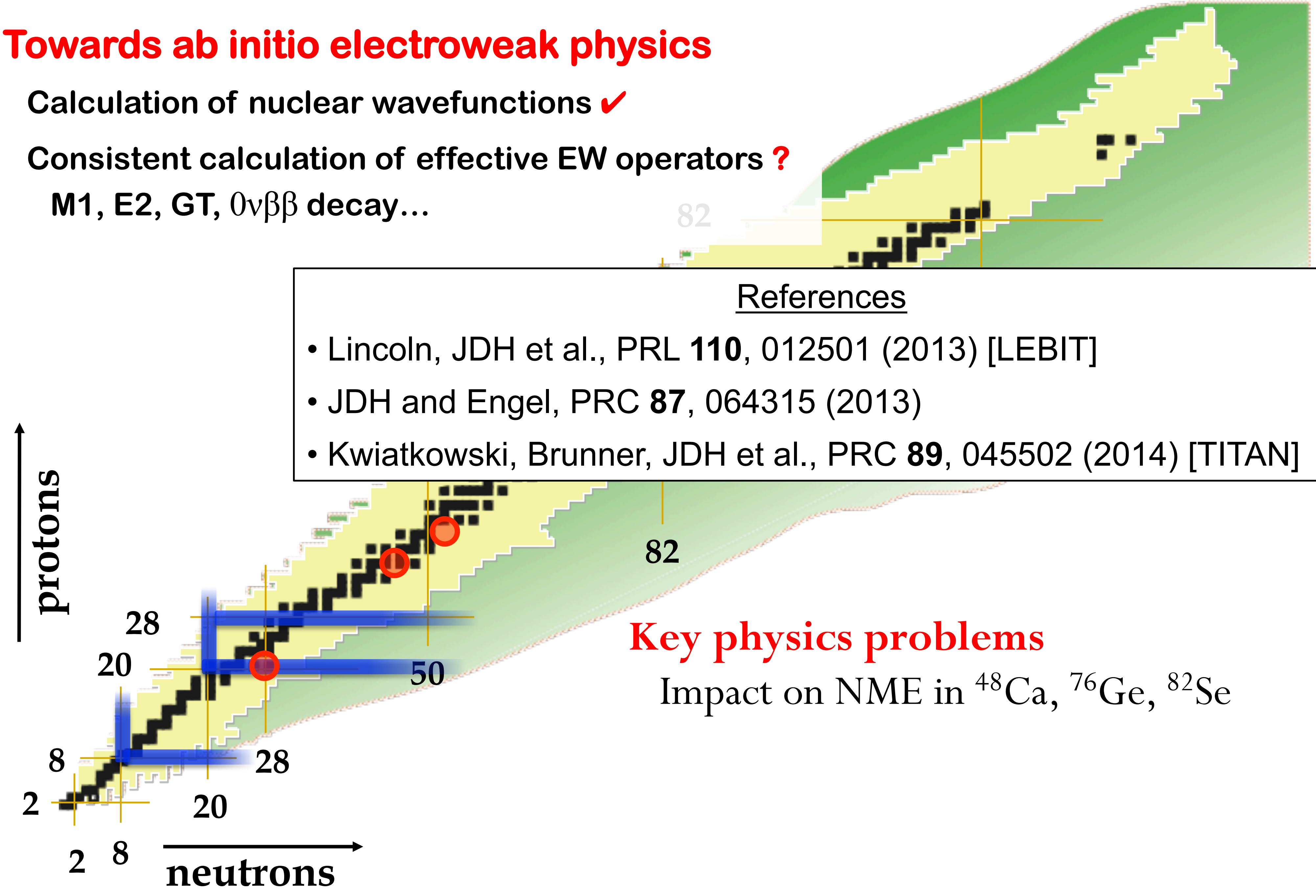
Calculations of Effective Operators (MBPT)

Towards ab initio electroweak physics

Calculation of nuclear wavefunctions ✓

Consistent calculation of effective EW operators ?

M1, E2, GT, 0νββ decay…



References

- Lincoln, JDH et al., PRL **110**, 012501 (2013) [LEBIT]
- JDH and Engel, PRC **87**, 064315 (2013)
- Kwiatkowski, Brunner, JDH et al., PRC **89**, 045502 (2014) [TITAN]

Key physics problems

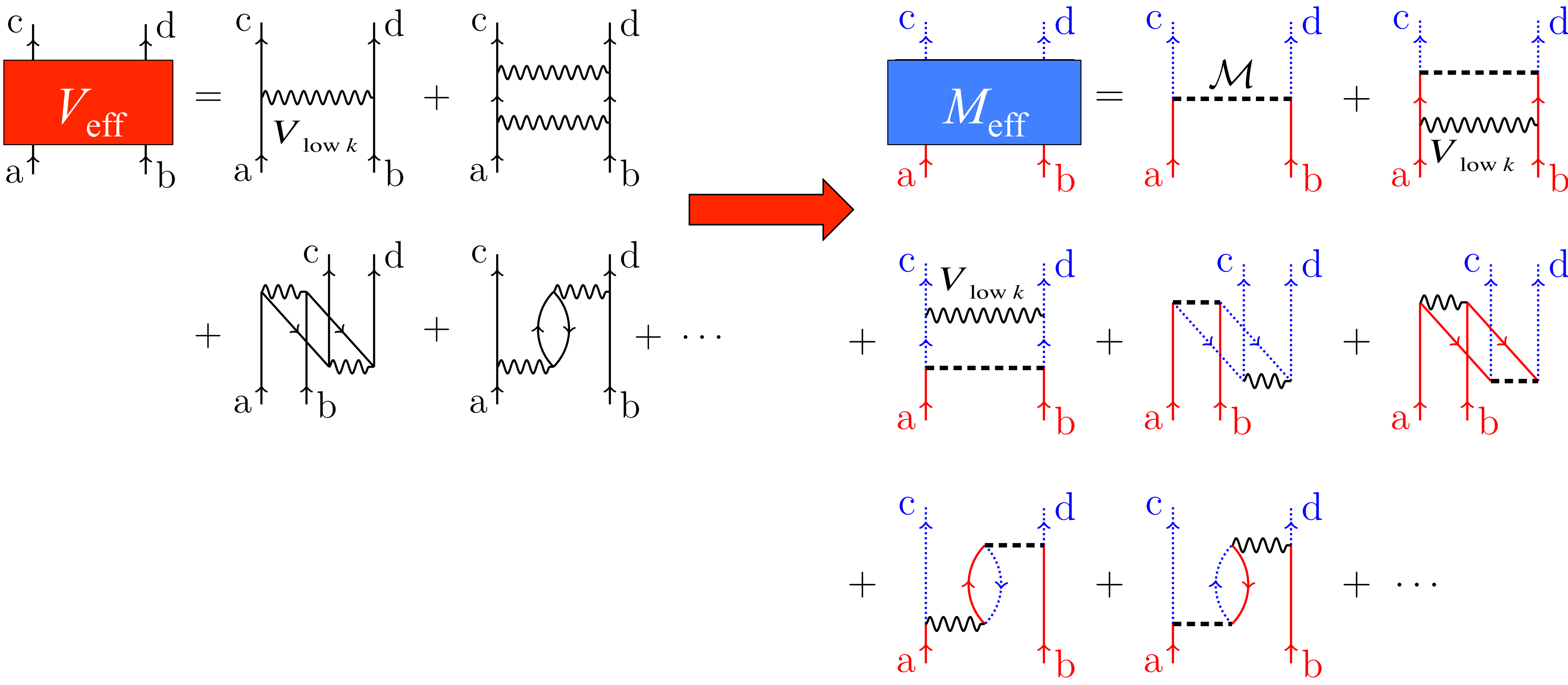
Impact on NME in ^{48}Ca, ^{76}Ge, ^{82}Se

Effective 0νββ-Decay Operator

Standard approach: phenomenological wavefunctions + **bare** operator

Calculate ***consistent effective*** 0νββ-decay operator using MBPT

Diagrammatically similar: replace one interaction vertex with $M_{0\nu}$ operator

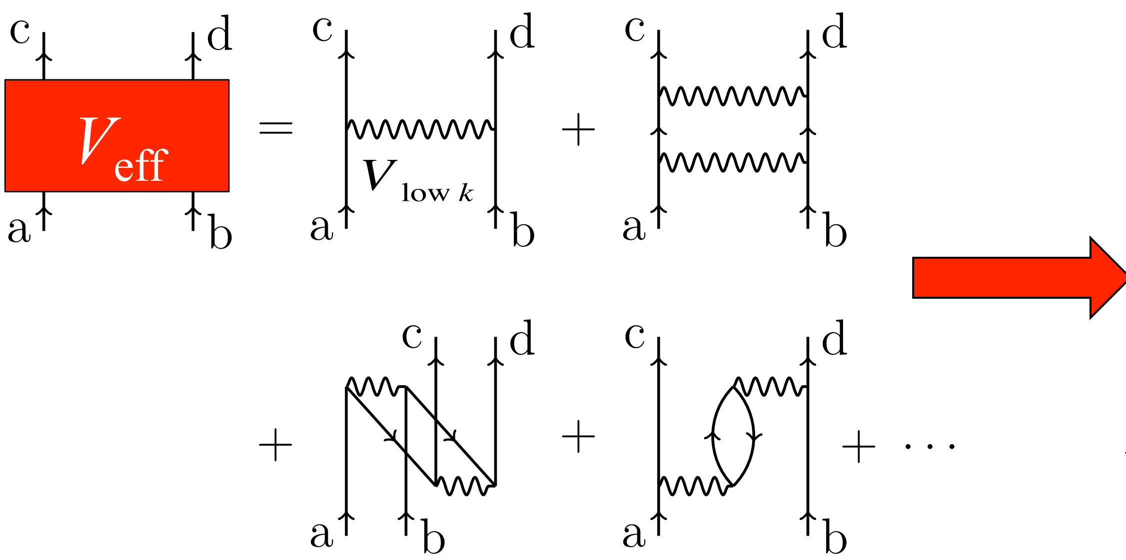


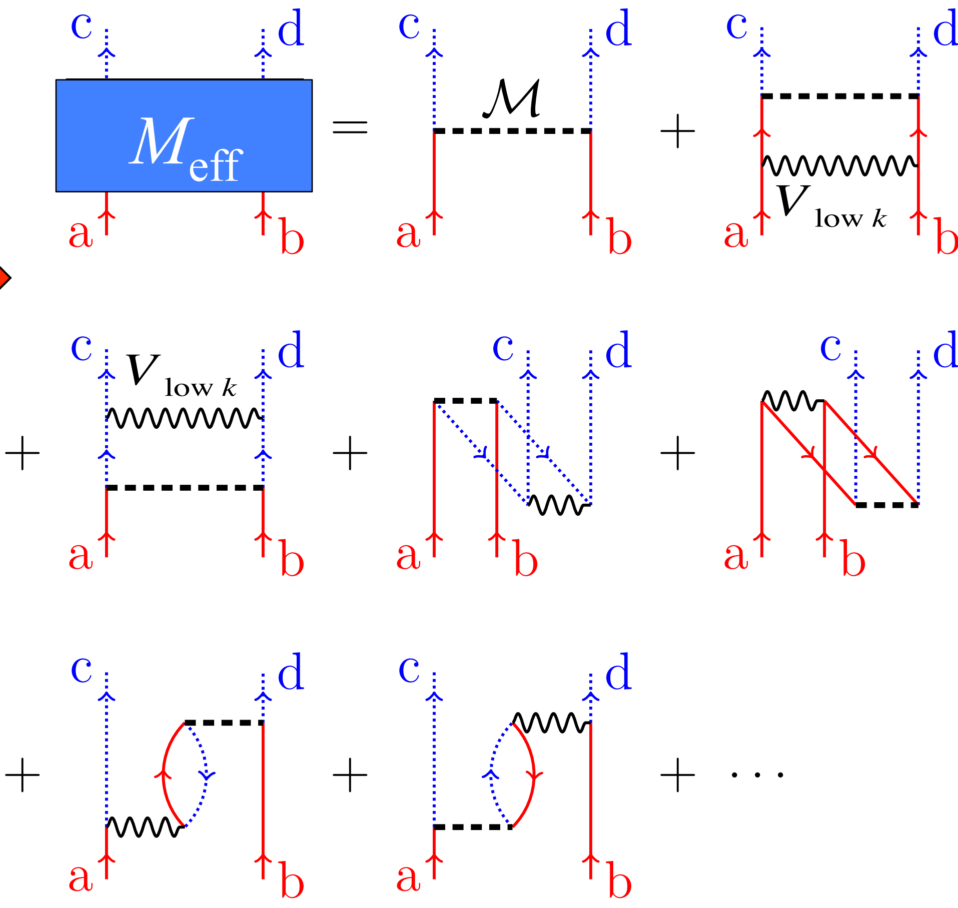
Effective 0νββ-Decay Operator

Standard approach: phenomenological wavefunctions + **bare** operator

Calculate ***consistent effective*** 0νββ-decay operator using MBPT

Diagrammatically similar: replace one interaction vertex with $M_{0\nu}$ operator





Previous: G-matrix calculation to

1^{st}-order MBPT non-convergent

Engel and Hagen, PRC (2009)

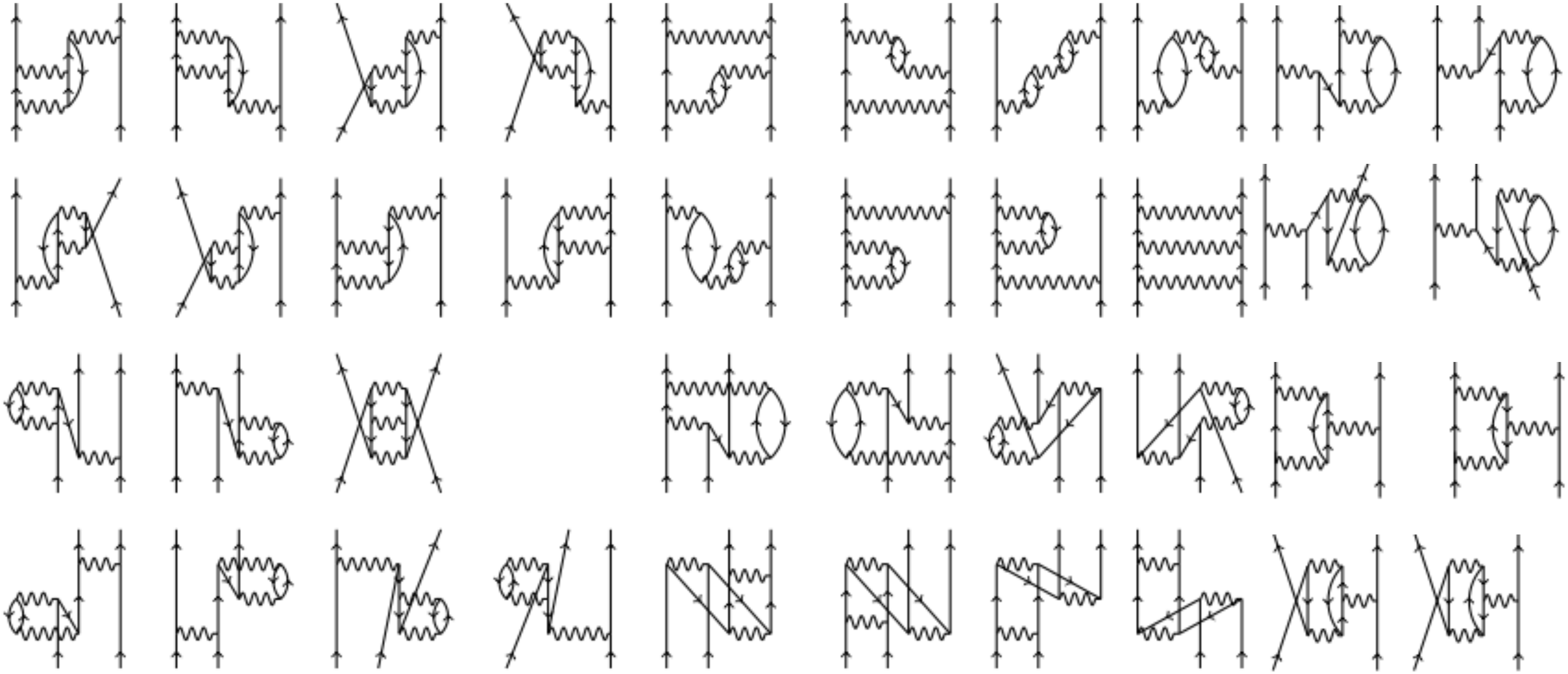
Low-momentum interactions: Improve convergence behavior?

Effective 0νββ-Decay Operator

Calculate in MBPT:

1st order (× 2)

2nd order (×3)



Calculations of $M_{0\nu}$ in ^{48}Ca, ^{76}Ge, and ^{82}Se

Phenomenological wavefunctions from A. Poves, M. Horoi

^{48}Ca	Bare	**0.77**
	Effective	**1.30**

^{76}Ge	Bare	**3.12**
	Effective	**3.77**

^{82}Se	Bare	**2.73**
	Effective	**3.62**

Converged in 13 major oscillator shells

No order-by-order convergence in MBPT

Lincoln, JDH et al., PRL (2013)
JDH and Engel, PRC (2013)
Kwiatkowski, et al., PRC (2014)

Overall ~25-30% increase for ^{76}Ge, ^{82}Se; 75% for ^{48}Ca

Calculations of $M_{0\nu}$ in ^{48}Ca, ^{76}Ge, and ^{82}Se

Phenomenological wavefunctions from A. Poves, M. Horoi

^{48}Ca	Bare	**0.77**
	Effective	**1.30**

^{76}Ge	Bare	**3.12**
	Effective	**3.77**

^{82}Se	Bare	**2.73**
	Effective	**3.62**

Converged in 13 major oscillator shells

No order-by-order convergence in MBPT

Lincoln, JDH et al., PRL (2013)

JDH and Engel, PRC (2013)

Kwiatkowski, et al., PRC (2014)

Overall ~25-30% increase for ^{76}Ge, ^{82}Se; 75% for ^{48}Ca

Promising first steps – up next…

- Consistent wavefunctions and operators in MBPT from chiral NN+3N
- Operator corrections: two-body currents from chiral EFT
- Nonperturbative methods (IM-SRG)
- Effects of induced 3-body operators

Calculations of $M_{0\nu}$ in ^{48}Ca, ^{76}Ge, and ^{82}Se

Phenomenological wavefunctions from A. Poves, M. Horoi

^{48}Ca	Bare	**0.77**
	Effective	**1.30**

^{76}Ge	Bare	**3.12**
	Effective	**3.77**

^{82}Se	Bare	**2.73**
	Effective	**3.62**

Converged in 13 major oscillator shells

No order-by-order convergence in MBPT

Lincoln, JDH et al., PRL (2013)
JDH and Engel, PRC (2013)
Kwiatkowski, et al., PRC (2014)

Overall ~25-30% increase for ^{76}Ge, ^{82}Se; 75% for ^{48}Ca

Promising first steps – up next…

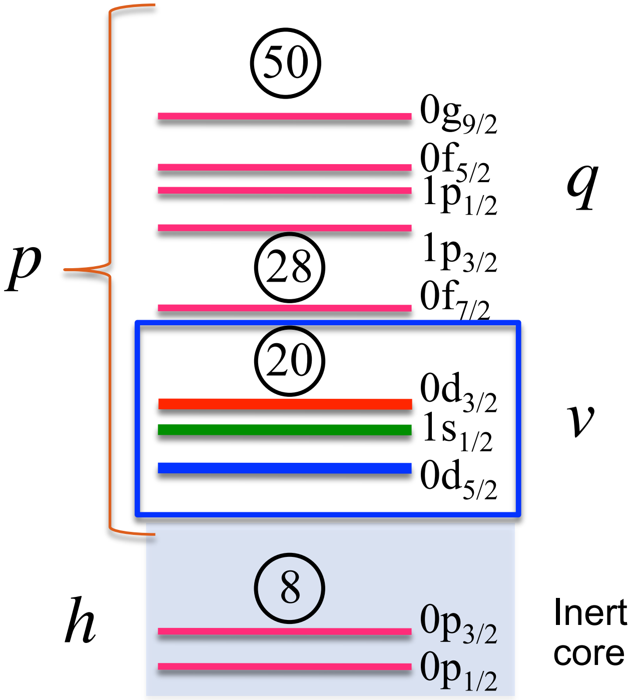
- Consistent wavefunctions and operators in MBPT from chiral NN+3N
- Operator corrections: two-body currents from chiral EFT
- **Nonperturbative methods (IM-SRG)**
- **Effects of induced 3-body operators**

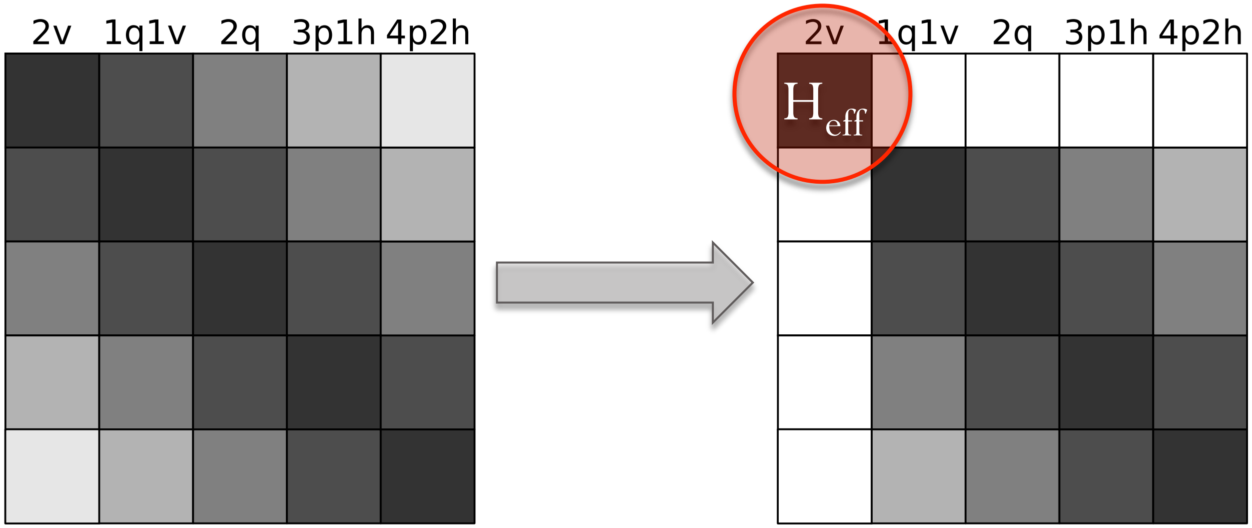
IM-SRG for Valence-Space Hamiltonians

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

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

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





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

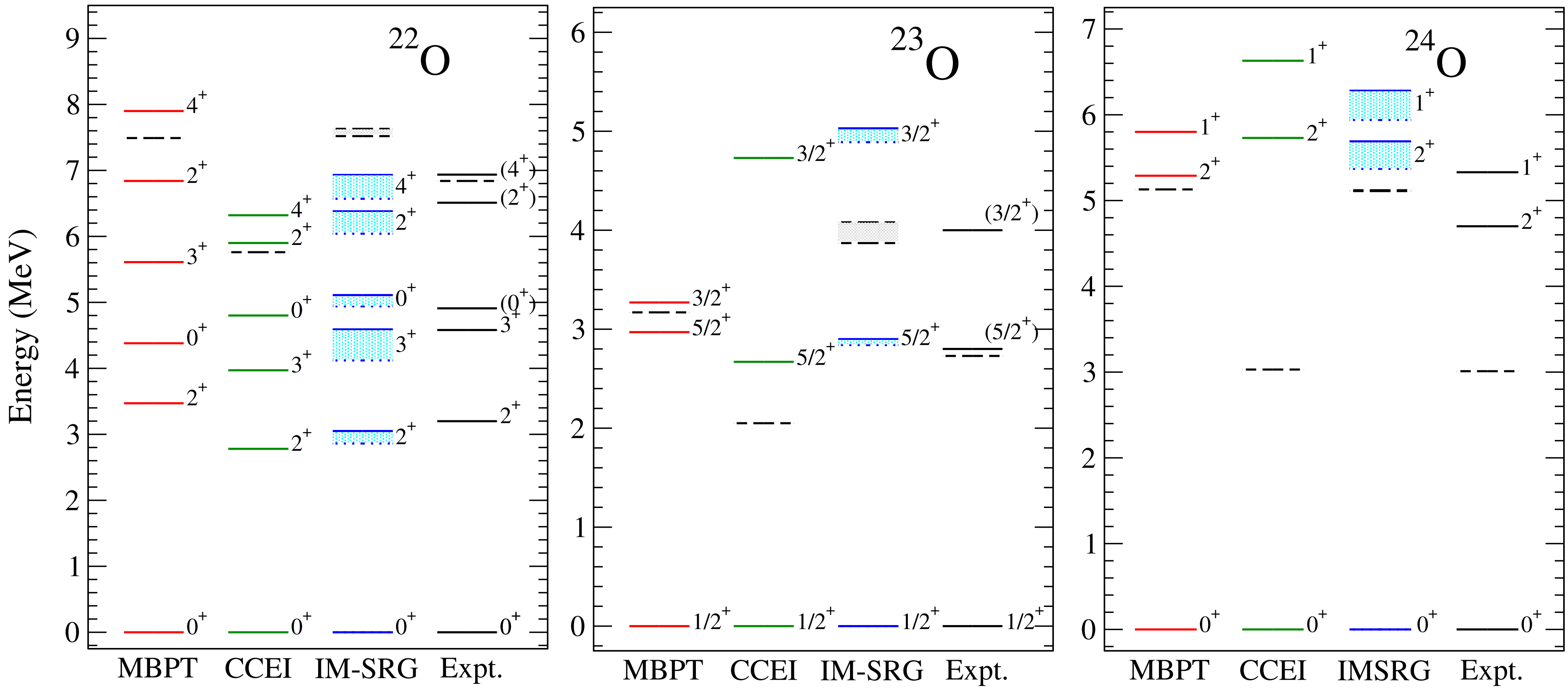
Separate p states into valence states (v) and those above valence space (q)

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

First nonperturbative construction of valence-space Hamitonians: H_{eff}

Benchmark in Oxygen with MBPT/CCEI

Compare with **Coupled-Cluster** effective interactions from NN+3N forces



Bogner, Hergert, JDH, Schwenk et al., PRL (2014)

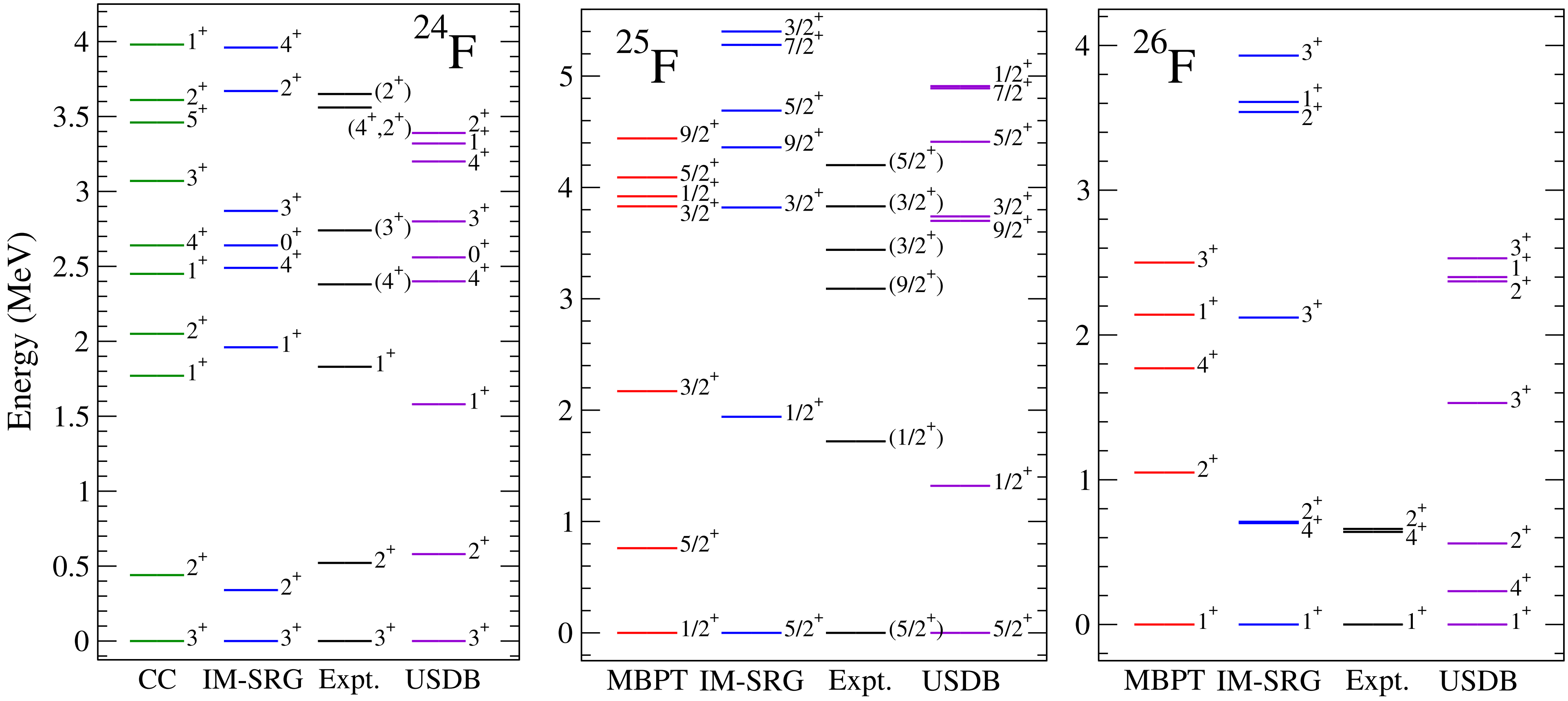
Hebeler, JDH, Menéndez, Schwenk, ARNPS (2015)

Many-Body Perturbation Theory in extended valence space ($sdf_{7/2}p_{3/2}$)

IM-SRG/**CCEI** (*sd* shell) spectra agree within ~300 keV; improved quality

Fully Open Shell: Neutron-Rich Fluorine Spectra

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



Bogner, Hergert, JDH, Schwenk, in prep.

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

Preliminary results already for scalar operators: charge radii, E0 transitions

Upcoming: general operators M1, E2, GT, double-beta decay Stroberg et al.

Effective Operators

Calculate unitary transformation directly

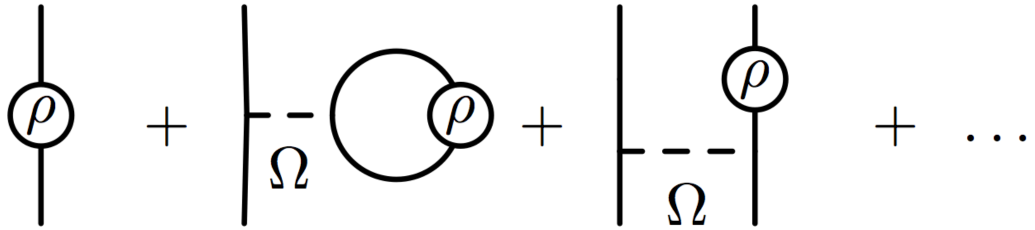
$$H(s) = e^{\Omega(s)} H e^{-\Omega(s)} = H + \frac{1}{2}[\Omega(s), H] + \frac{1}{12}[\Omega(s), [\Omega(s), H]] + \cdots$$

Straightforward to generalize to arbitrary operators

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

First apply to scalar operators: charge radii, E0 transitions

Commutators induce important higher-order one-/two-body parts

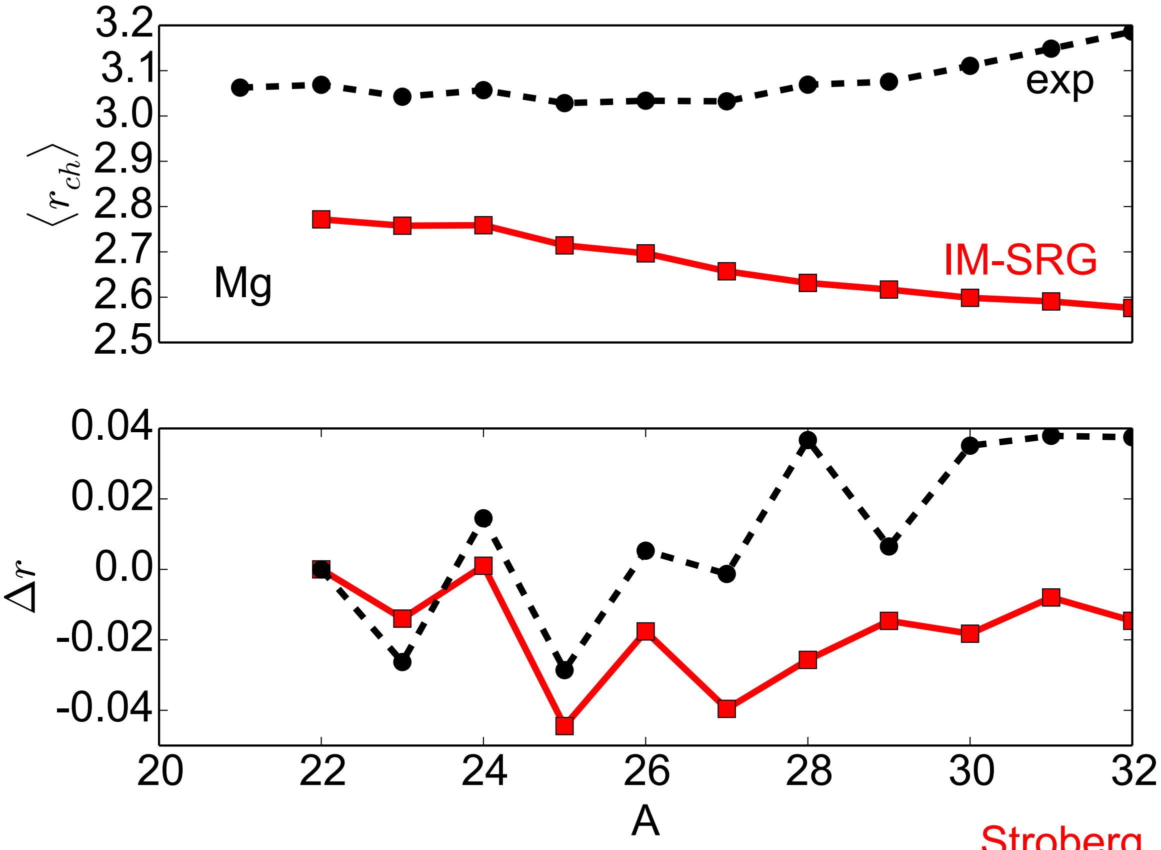


Quantify importance of induced higher-body contributions!

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%

Path to Full Calculation

Consistent wavefunction and operator

SRG-evolved operator Shuster et al.

Improvements in operator

Two-body currents from chiral EFT

Menendez, Gazit, Schwenk, PRL (2011)

Ekstrom, Wendt, et al., PRL (2014)

Exotic decay mechanisms Horoi

Heavier candidates accessible to SM

Importance of spin-orbit partners

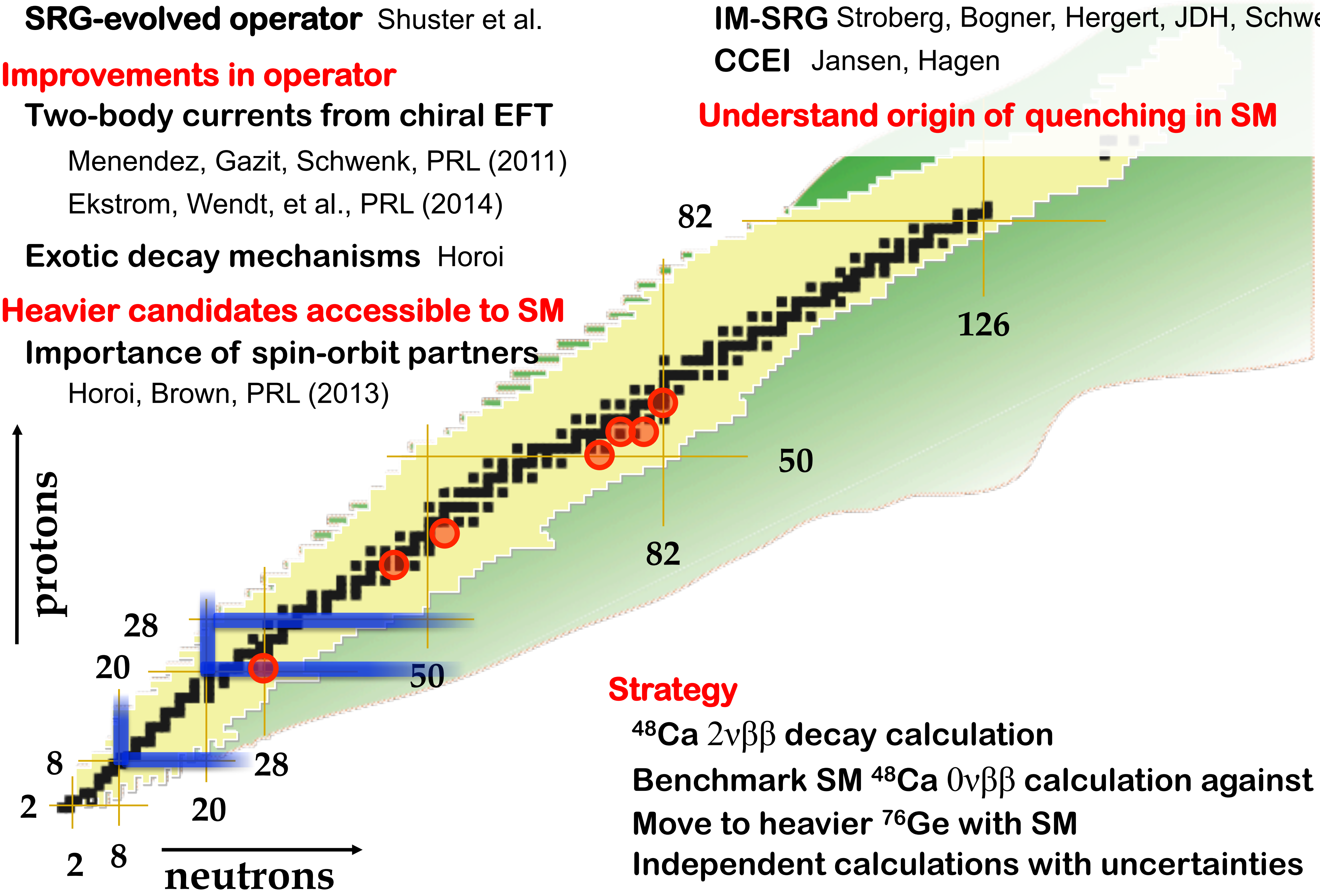
Horoi, Brown, PRL (2013)

Nonperturbative SM wfs/operators

IM-SRG Stroberg, Bogner, Hergert, JDH, Schwenk

CCEI Jansen, Hagen

Understand origin of quenching in SM



Strategy

^{48}Ca $2\nu\beta\beta$ decay calculation

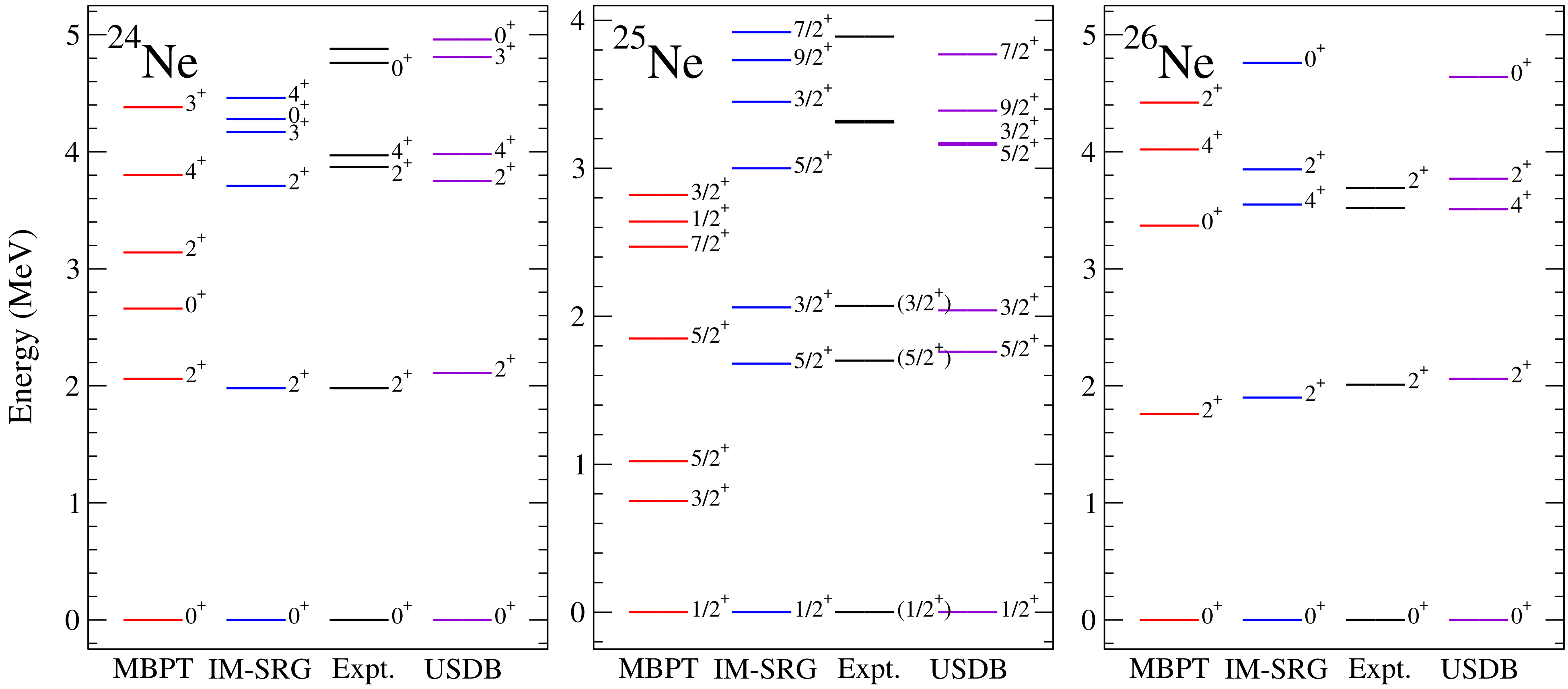
Benchmark SM ^{48}Ca $0\nu\beta\beta$ calculation against CC

Move to heavier ^{76}Ge with SM

Independent calculations with uncertainties

Fully Open Shell: Neutron-Rich Neon Spectra

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



Bogner, Hergert, JDH, Schwenk, in prep.

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

Preliminary results already for scalar operators: charge radii, E0 transitions

Upcoming: general operators M1, E2, GT, double-beta decay R. Stroberg et al.

0νββ-Decay Operator

Details of operator used in subsequent calculations

Closure approximation good to 8-10% Sen’kov, Horoi, Brown, PRC (2014)

$$M_{0\nu} = \frac{2R}{\pi g_A^2}\int_0^\infty q\,dq$$

$$\times \langle f|\sum_{a,b}\frac{j_0(qr_{ab})[h_F(q)+h_{GT}(q)\vec{\sigma}_a\cdot\vec{\sigma}_b]}{q+\overline{E}-(E_i+E_f)/2}\tau_a^+\tau_b^+\,|i\rangle$$

$$h_F(q) \equiv -g_V^2(q^2),$$

$$h_{GT}(q) \equiv g_A^2(q^2) - \frac{g_A(q^2)g_P(q^2)q^2}{3m_p} + \frac{g_P^2(q^2)q^4}{12m_p^2} + \frac{g_M^2(q^2)q^2}{6m_p^2}$$

$$g_V(q^2) = \frac{1}{[1+q^2/(0.85\mathrm{GeV}^2)]^2} \qquad g_P(q^2) = \frac{2m_p g_A(q^2)}{q^2+m_\pi^2}$$

$$g_A(q^2) = \frac{1.27}{[1+q^2/(1.09\mathrm{Gev}^2)]^2}, \qquad g_M(q^2) = 3.70 g_V(q^2)$$

1) Nuclear wavefunctions: currently phenomenological – calculate ab initio
2) **Decay operator**: **correlations outside valence space**; 2-body currents

Calculations of $M_{0\nu}$ in ^{82}Se and ^{76}Ge

Phenomenological wavefunctions from A. Poves, M. Horoi ($pf_{5/2}\,g_{9/2}$ space)

^{76}Ge	Bare matrix element	**3.12**
	Full 1st order	**3.11**
	Full 2nd order	**3.77**

^{82}Se	Bare matrix element	**2.73**
	Full 1st order	**2.79**
	Full 2nd order	**3.62**

Lincoln, JDH et al., PRL (2013) [LEBIT]

JDH and Engel, PRC (2013)

Converged in 13 major oscillator shells

Little net effect at 1st order – no clear order-by-order convergence

Overall ~25-30% increase from bare value

Calculations of $M_{0\nu}$ in ^{48}Ca

Phenomenological wavefunctions from GXPF1A (*pf* shell)

^{48}Ca	GT	Fermi	Tensor	**Sum**
Bare	0.675	0.130	−0.072	**0.733**
Final	1.211	0.160	−0.070	**1.301**

Kwiatkowski, JDH, Engel, Horoi et al., PRC (2014)

Converged in 13 major oscillator shells

Similar absolute increase as in Ge, Se – no clear order-by-order convergence

Overall ~75% increase from bare value

Calculations of $M_{0\nu}$ in ^{48}Ca

Phenomenological wavefunctions from GXPF1A (*pf* shell)

^{48}Ca	GT	Fermi	Tensor	**Sum**
Bare	0.675	0.130	−0.072	**0.733**
Final	1.211	0.160	−0.070	**1.301**

Kwiatkowski, JDH, Engel, Horoi et al., PRC (2014)

Converged in 13 major oscillator shells

Similar absolute increase as in Ge, Se – no clear order-by-order convergence

Overall ~75% increase from bare value

Promising first steps – up next…

- Consistent wavefunctions and operators in MBPT from chiral NN+3N
- Operator corrections: two-body currents from chiral EFT
- Nonperturbative methods (IM-SRG)
- Effects of induced 3-body operators

Calculations of $M_{0\nu}$ in ^{48}Ca

Phenomenological wavefunctions from GXPF1A (*pf* shell)

^{48}Ca	GT	Fermi	Tensor	**Sum**
Bare	0.675	0.130	−0.072	**0.733**
Final	1.211	0.160	−0.070	**1.301**

Kwiatkowski, JDH, Engel, Horoi et al., PRC (2014)

Converged in 13 major oscillator shells

Similar absolute increase as in Ge, Se – no clear order-by-order convergence

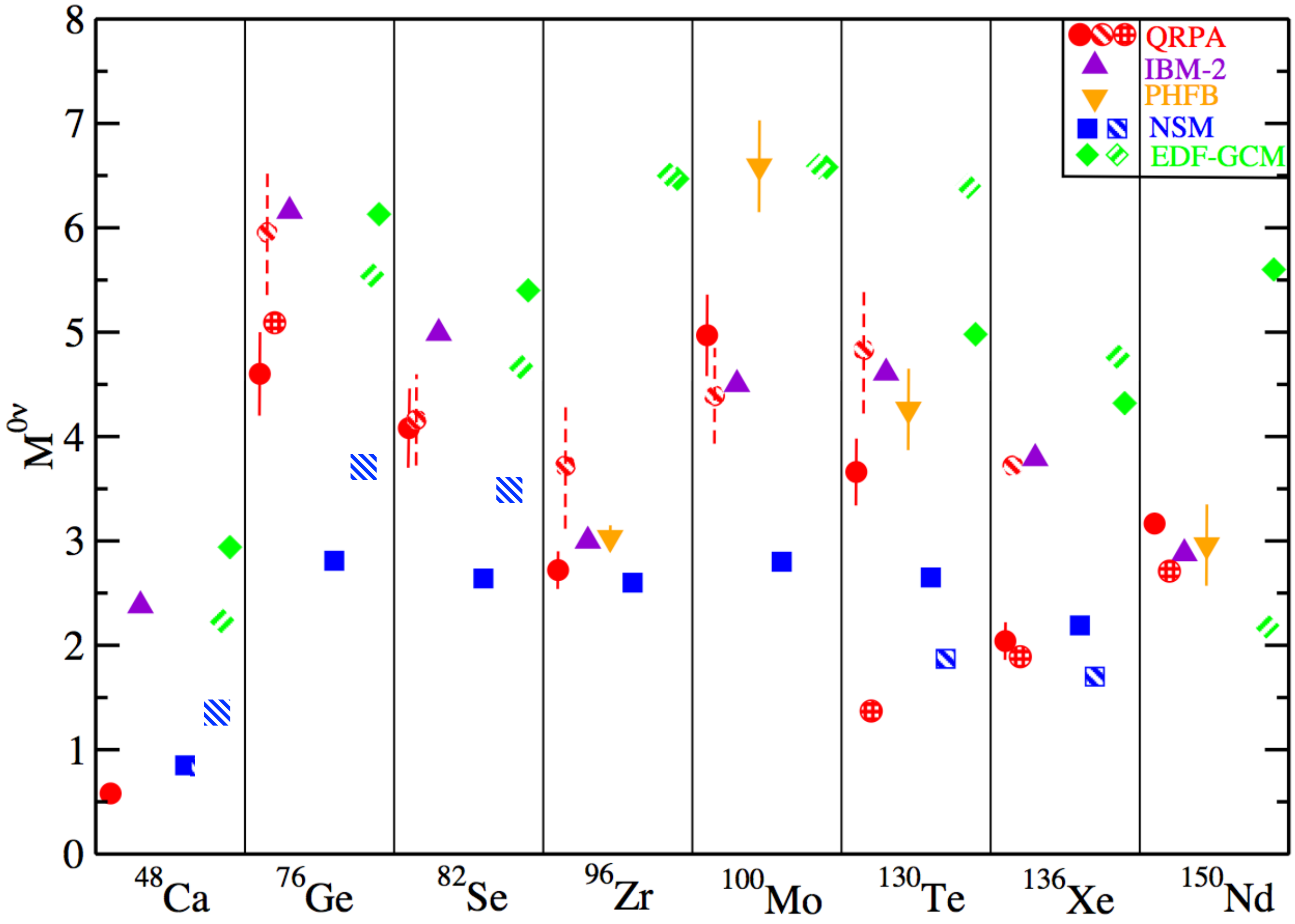
Overall ~75% increase from bare value

Promising first steps – up next…

- Consistent wavefunctions and operators in MBPT from chiral NN+3N
- Operator corrections: two-body currents from chiral EFT
- **Nonperturbative method for wavefunction and operator (IM-SRG)**
- **Effects of induced 3-body operators?**

Nuclear Matrix Element

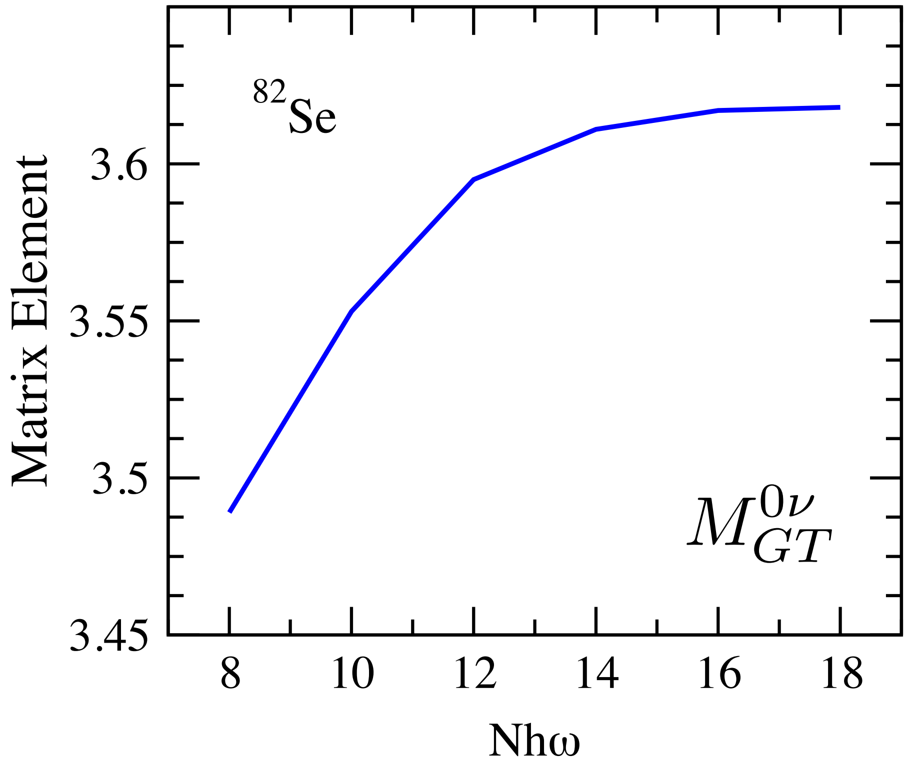
Improved calculations move in direction of other methods



Aim: first-principles framework capable of robust prediction

Intermediate-State Convergence

Convergence results in ^{82}Se



JDH and Engel, PRC (2013)

Results **well converged** in terms of intermediate state excitations

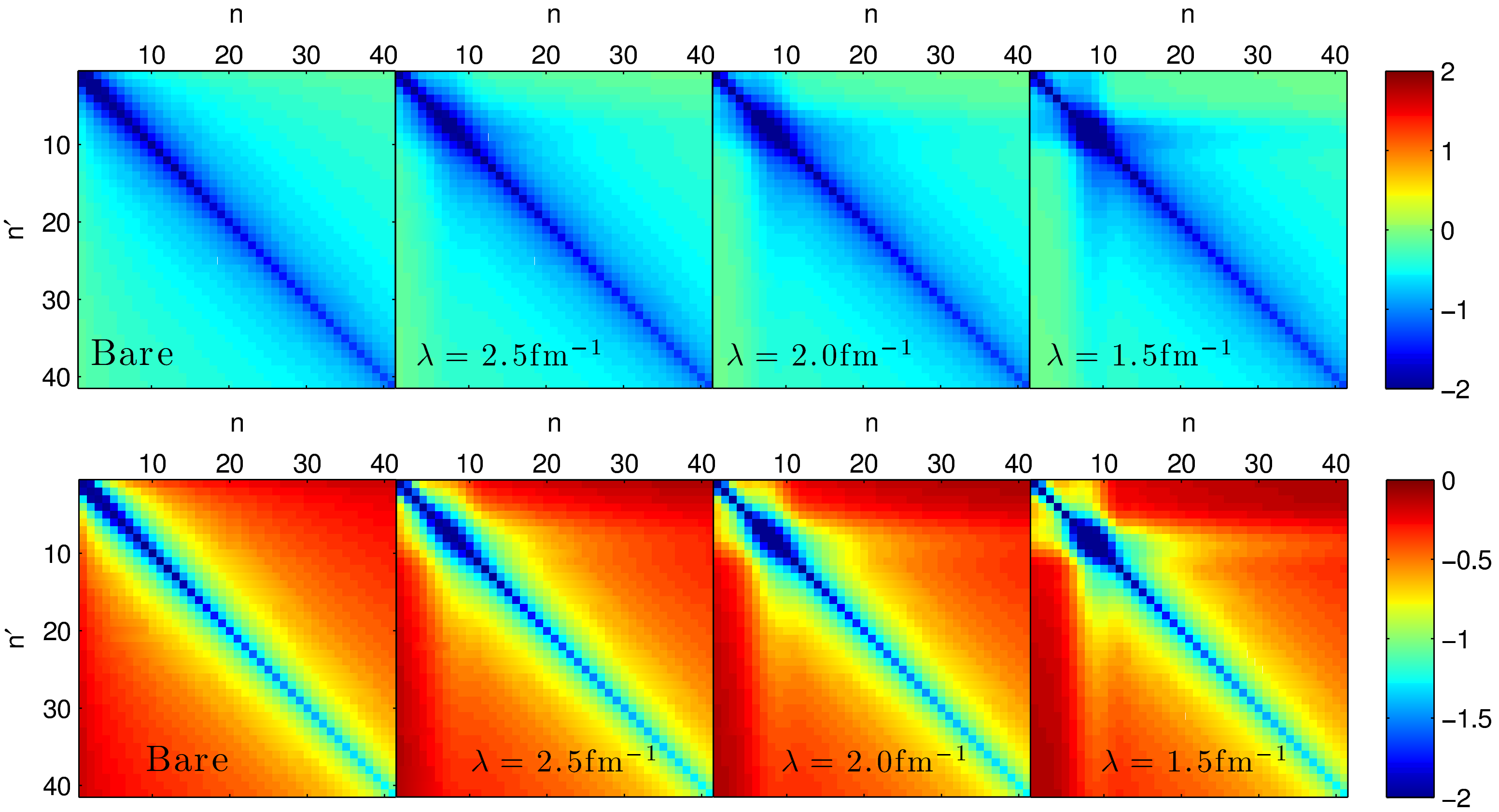
Improvement due to low-momentum interactions

Similar trend in ^{76}Ge and ^{48}Ca

Improvements from SRG-evolved operator?

SRG Evolution of Operator

Preliminary results with 0νββ-decay operator



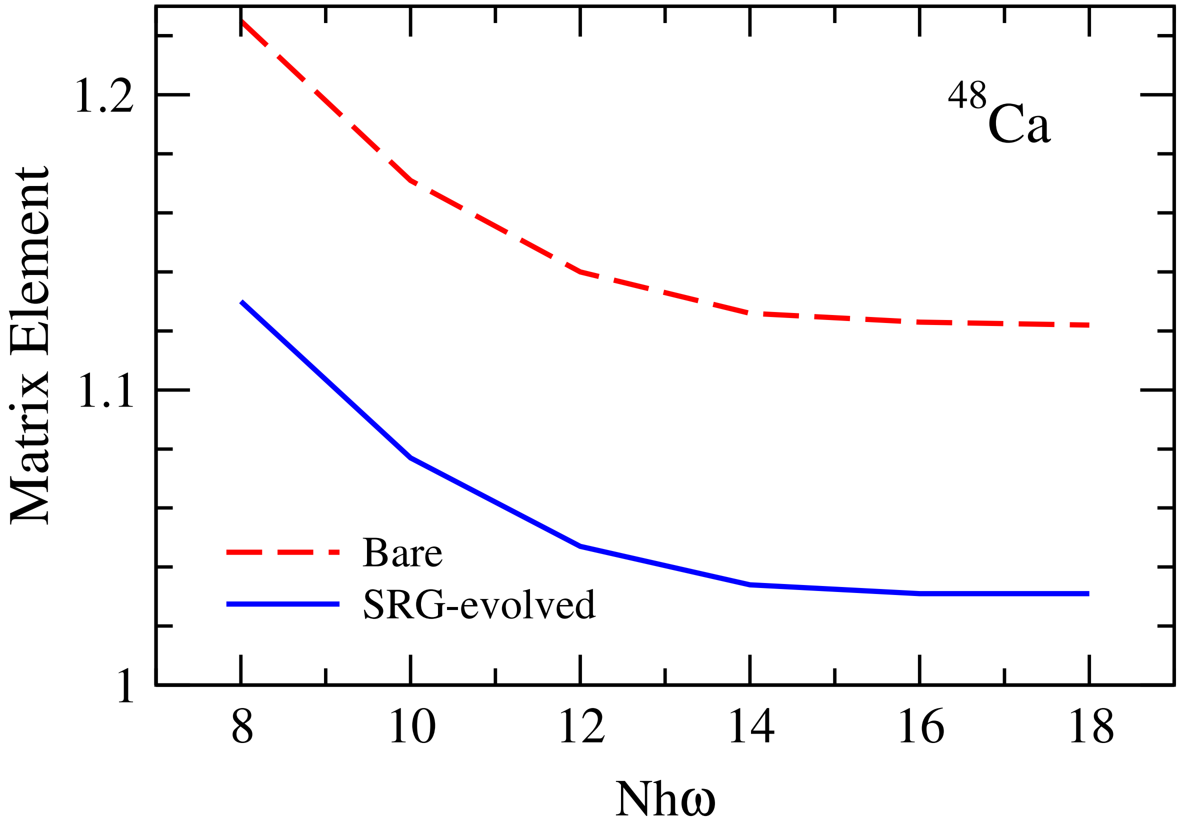
Schuster, Engel, JDH, Navrátil, Quaglioni

Minimal effects from SRG evolution

Negligible improvements in MBPT convergence?

SRG Evolution of Operator

Preliminary results with 0νββ-decay operator



Schuster, Engel, JDH, Navrátil, Quaglioni

Minimal improvement in intermediate-state convergence

Strategy

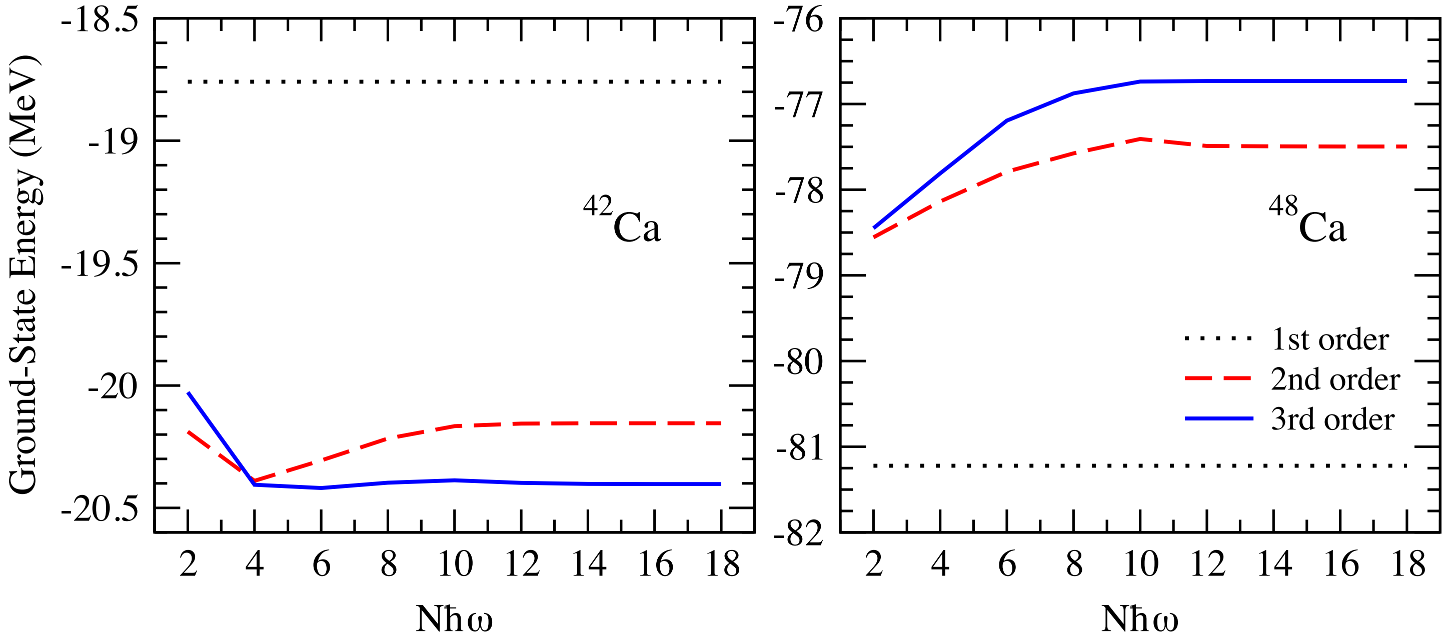
1) Effective interaction: sum excitations outside valence space to **3^{rd} order**

2) Single-particle energies calculated self-consistently

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

4) NN and 3N forces – fully to 3^{rd}-order MBPT

5) Work in extended valence spaces



Clear convergence with HO basis size

Promising order-by-order behavior

Strategy

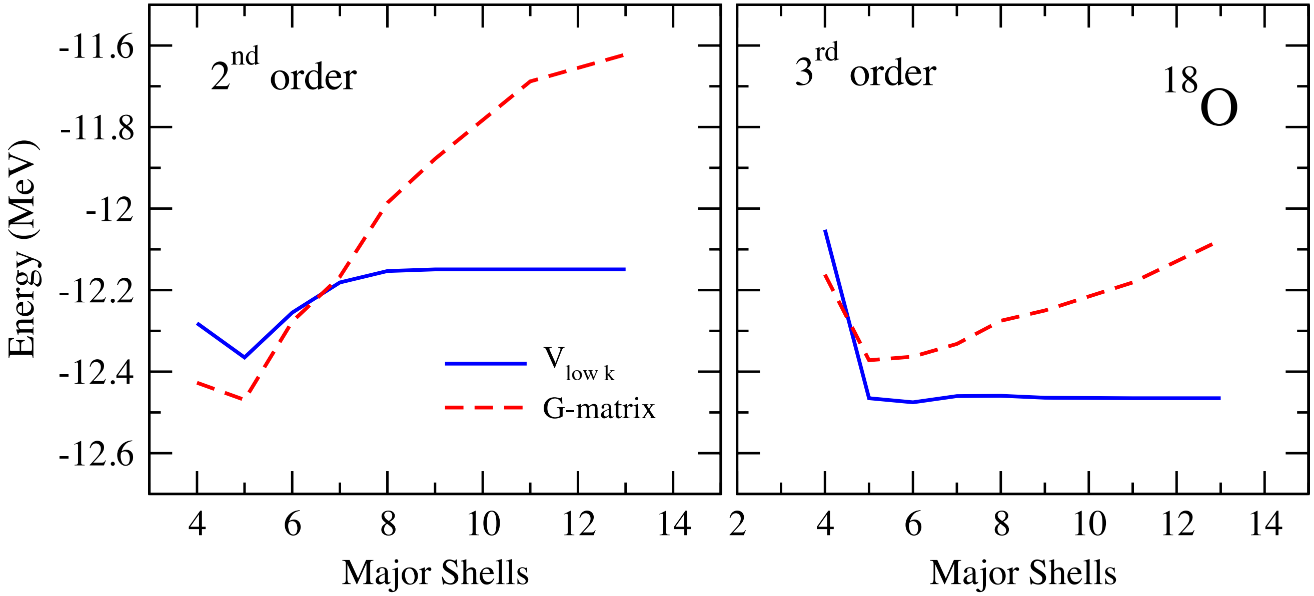
1) Effective interaction: sum excitations outside valence space to **3rd order**

2) Single-particle energies calculated self-consistently

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

4) NN and 3N forces – fully to 3rd-order MBPT

5) Work in extended valence spaces



G-matrix – no signs of convergence (similar in pf-shell)

Strategy

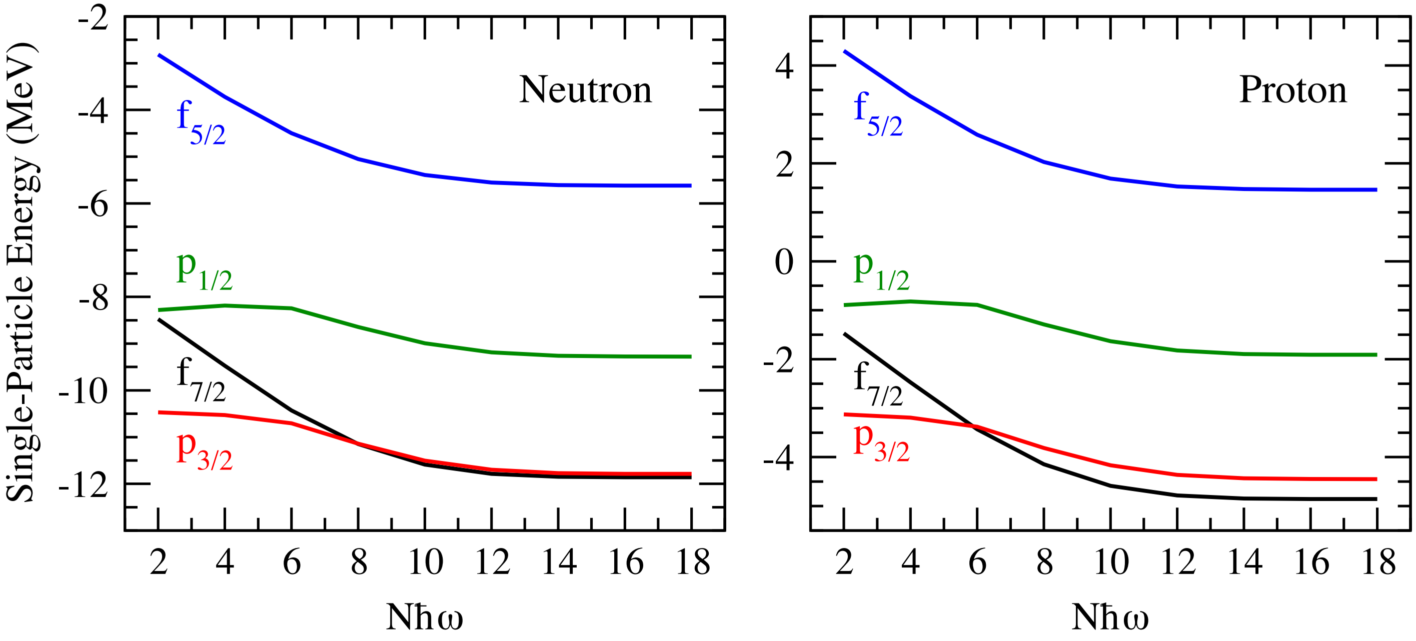
1) Effective interaction: sum excitations outside valence space to **3rd order**

2) Single-particle energies calculated self-consistently

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

4) NN and 3N forces – fully to 3rd-order MBPT

5) Work in extended valence spaces



Clear convergence with HO basis size

Promising order-by-order behavior

Nonperturbative In-Medium SRG

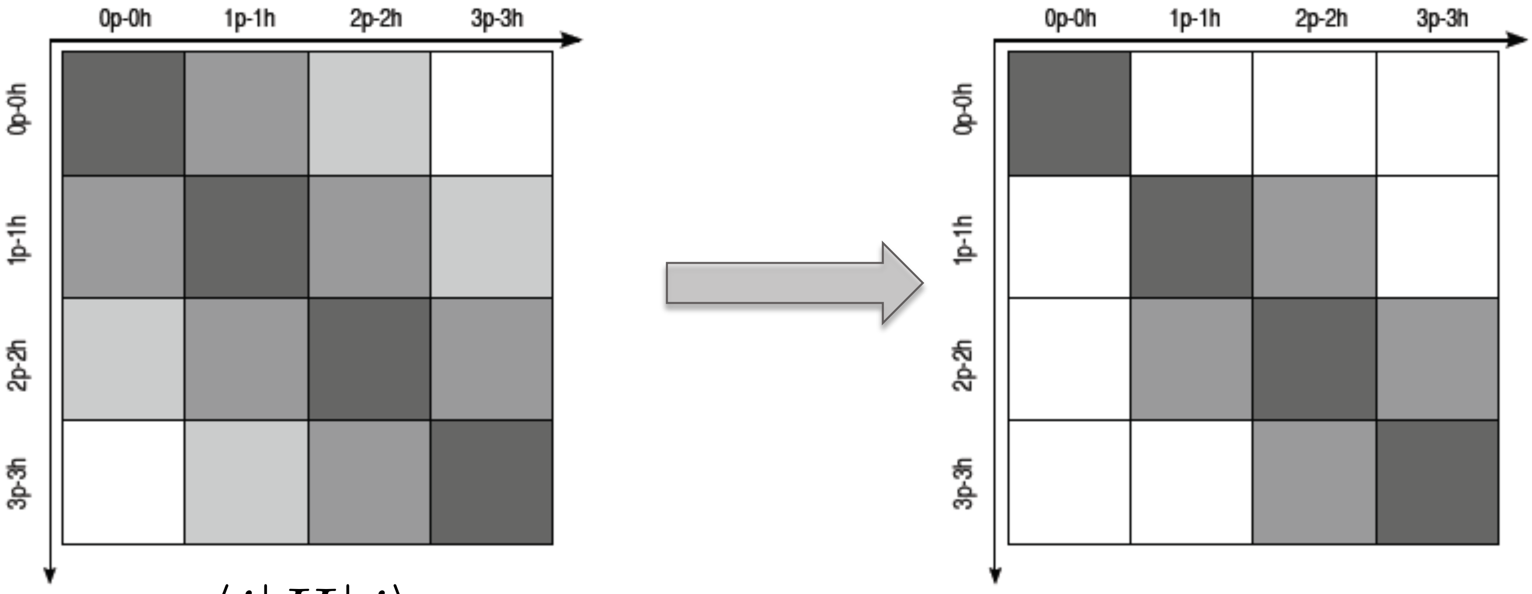
Tsukiyama, **Bogner**, Schwenk, PRL (2011)

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

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

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

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



$$\langle i|H|j\rangle$$

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

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)

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

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

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

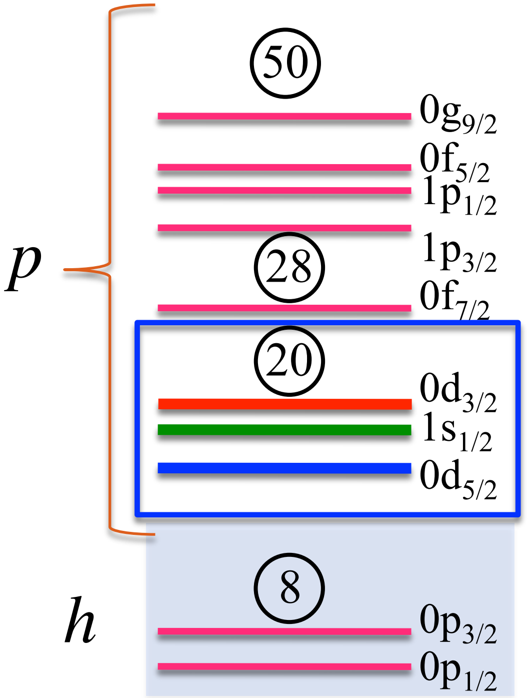
Ab initio method for energies of **closed-shell systems**

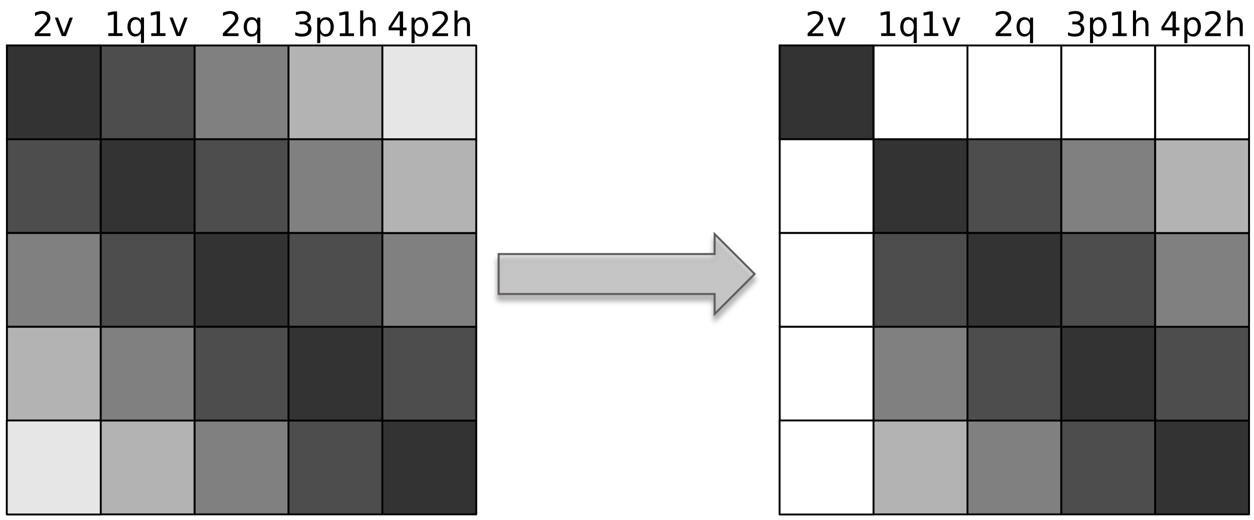
IM-SRG: Valence-Space Hamiltonians

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

Open-shell systems

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





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

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

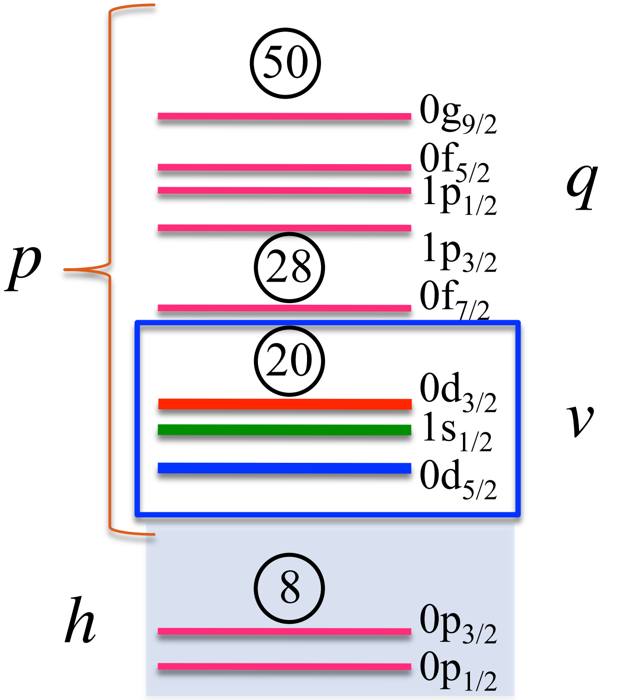
$$H^{\rm od} = \langle p|H|h\rangle + \langle pp|H|hh\rangle + \langle v|H|q\rangle + \langle pq|H|vv\rangle + \langle pp|H|hv\rangle + \text{h.c.}$$

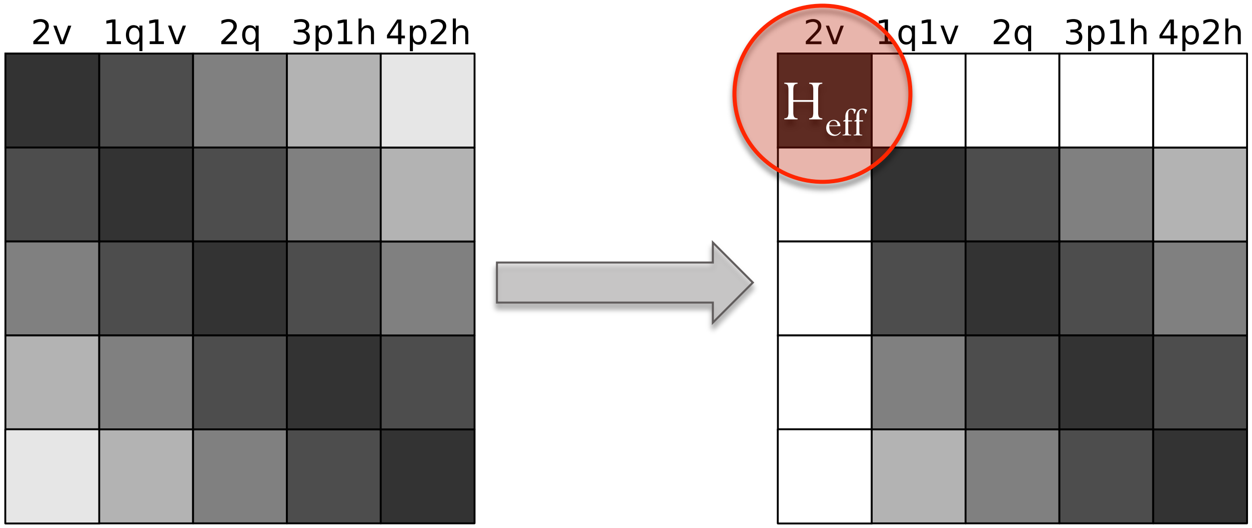
IM-SRG: Valence-Space Hamiltonians

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

Open-shell systems

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





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

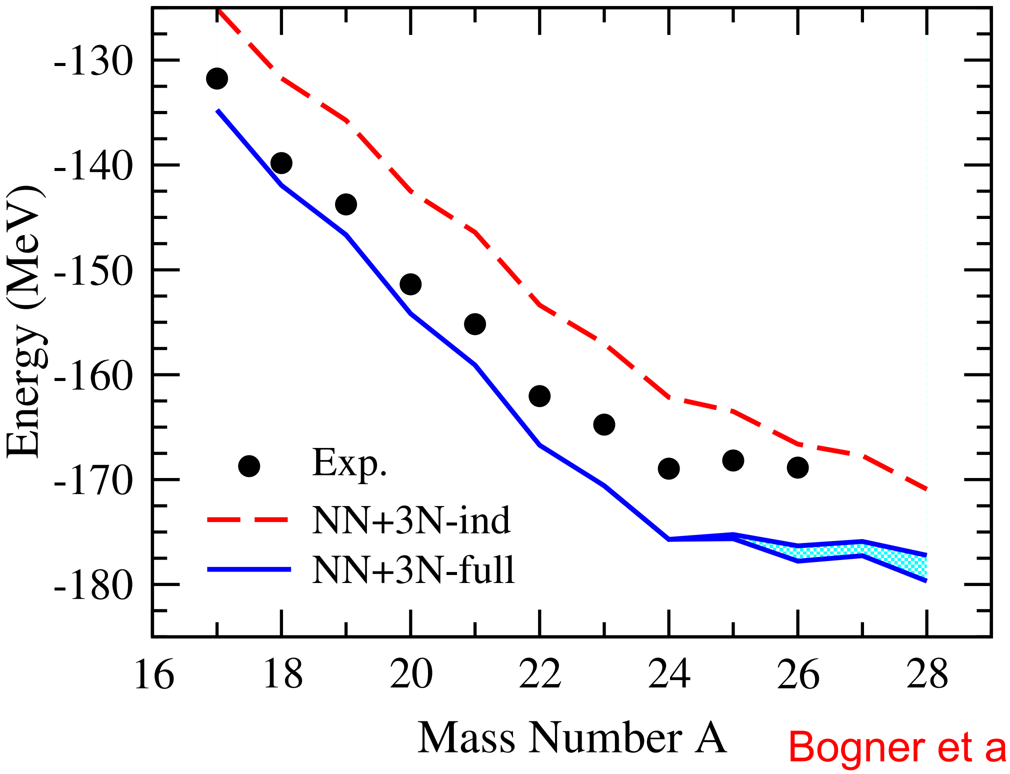
Core physics included consistently (**absolute energies, radii…**)

Inherently nonperturbative – no need for extended valence space

Non-degenerate valence-space orbitals

IM-SRG Oxygen Ground-State Energies

IM-SRG valence-space interaction and SPEs in *sd* shell



Bogner et al., PRL (2014)

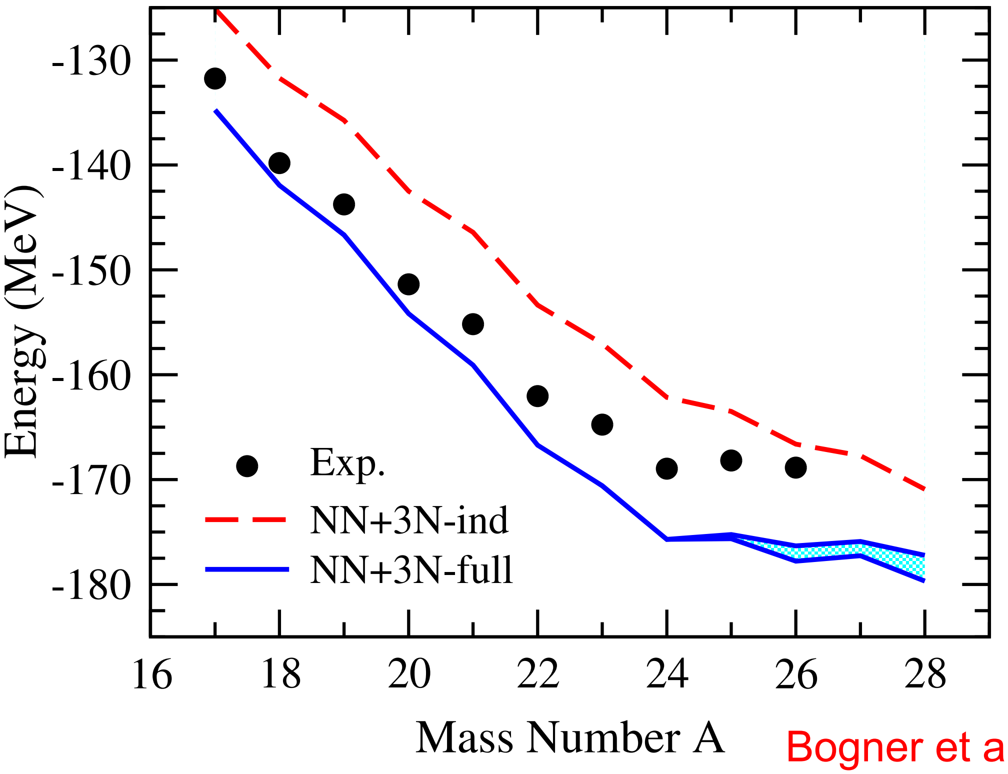
NN+3N-ind modest underbinding, dripline not reproduced

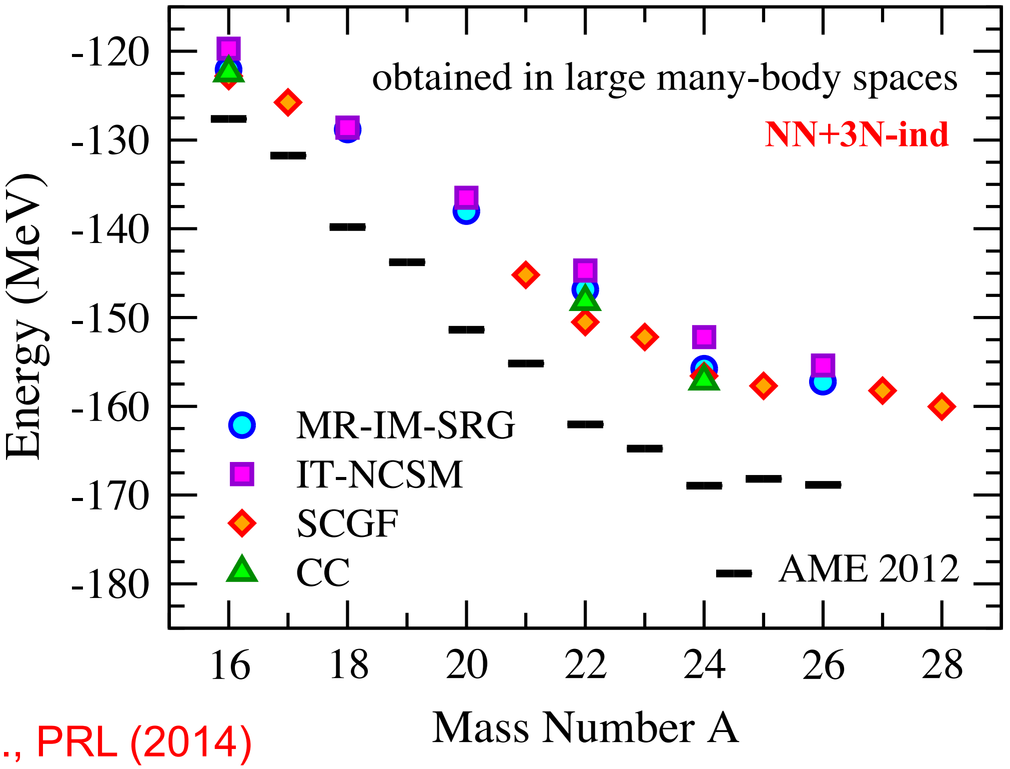
NN+3N-full modestly overbound, correct dripline trend

Weak $\hbar\omega$ dependence

Comparison with Large-Space Methods

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



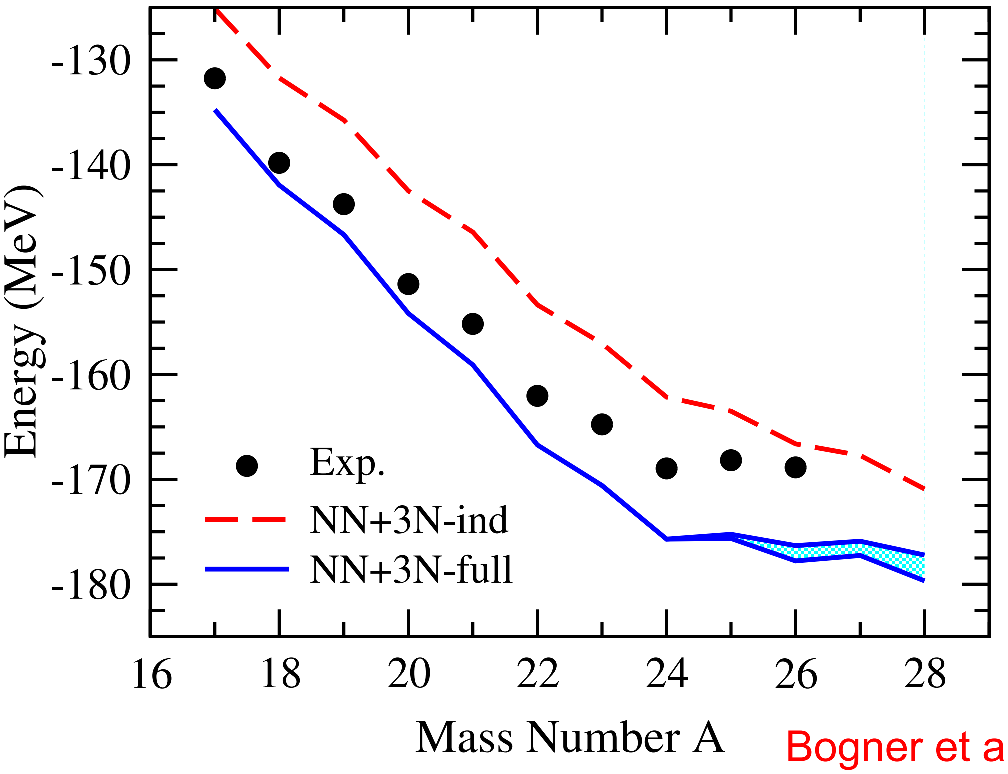


Bogner et al., PRL (2014)

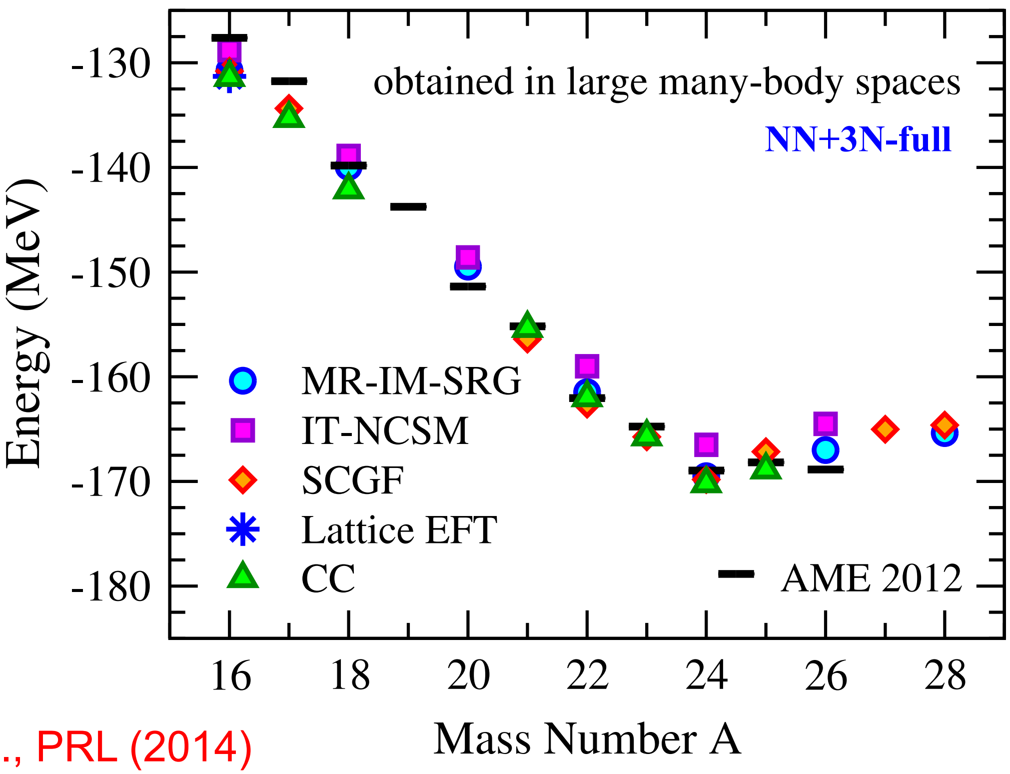
Agreement between all methods with same input forces

Comparison with Large-Space Methods

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



Bogner et al., PRL (2014)



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

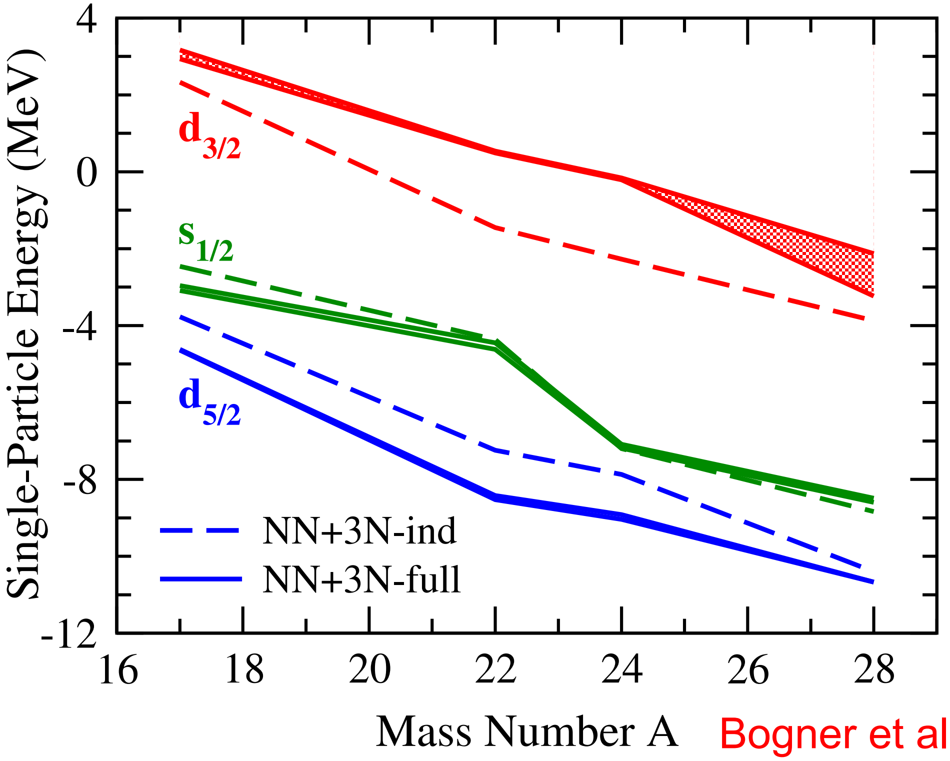
Agreement between all methods with same input forces

Clear improvement with NN+3N-full

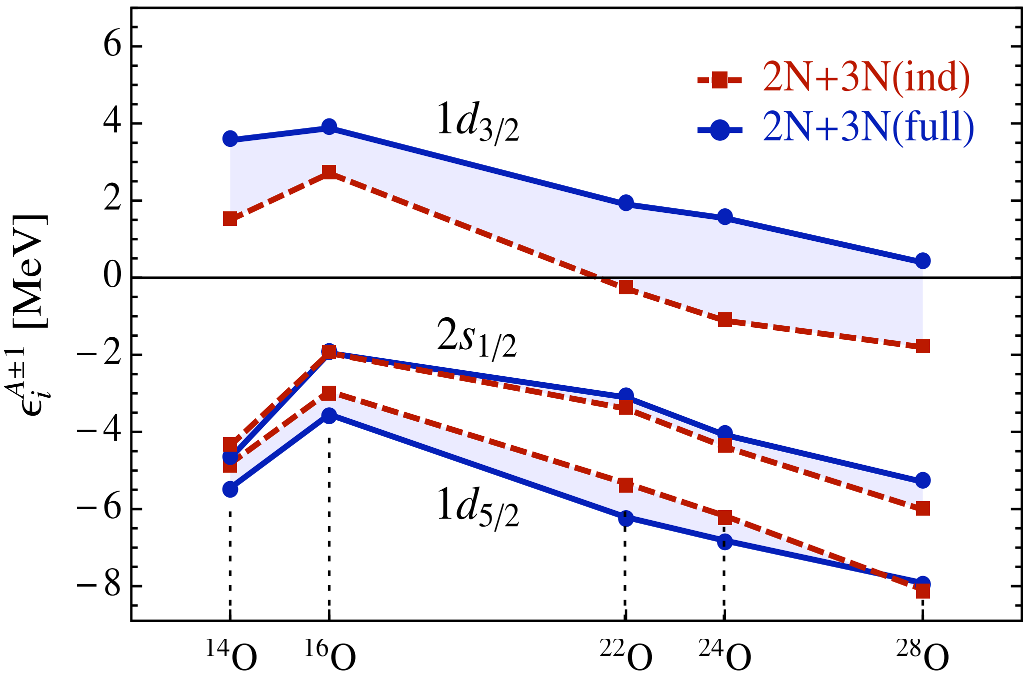
Validates valence-space results

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)

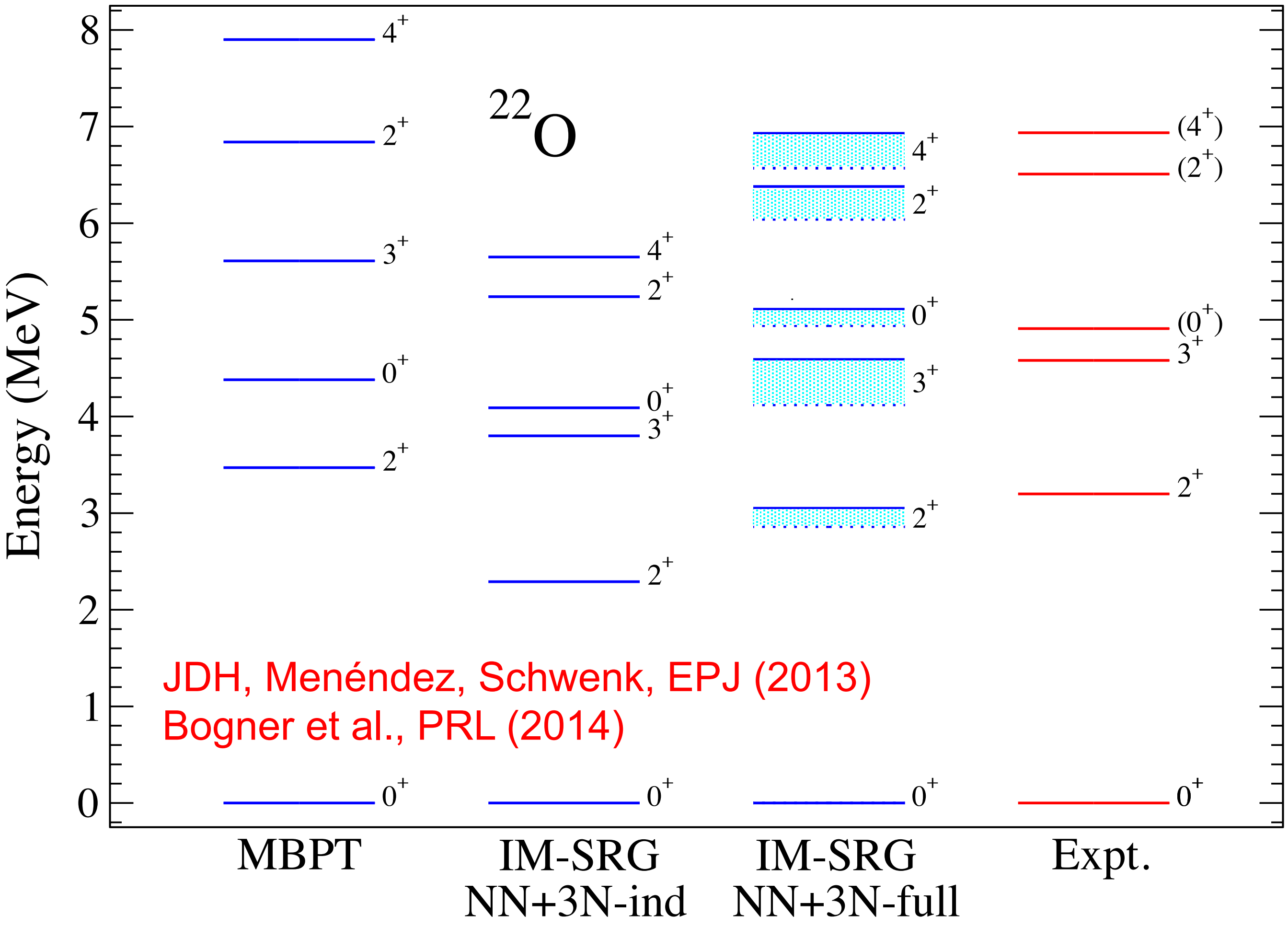
Robust mechanism driving dripline behavior

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



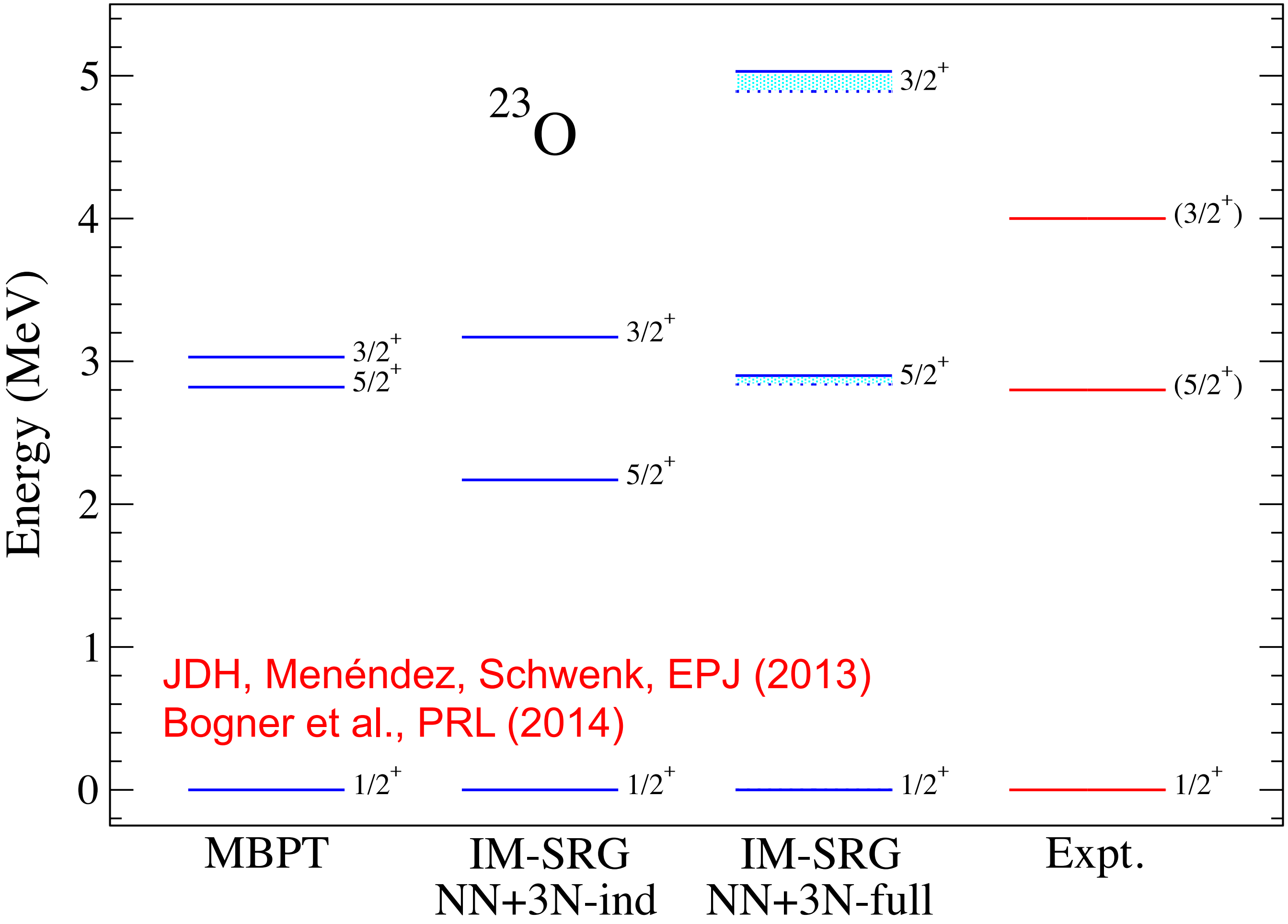
JDH, Menéndez, Schwenk, EPJ (2013)
Bogner et al., PRL (2014)

Clear improvement with NN+3N-full

IM-SRG: comparable with phenomenology

IM-SRG Oxygen Spectra

Oxygen spectra: extended-space MBPT and IM-SRG

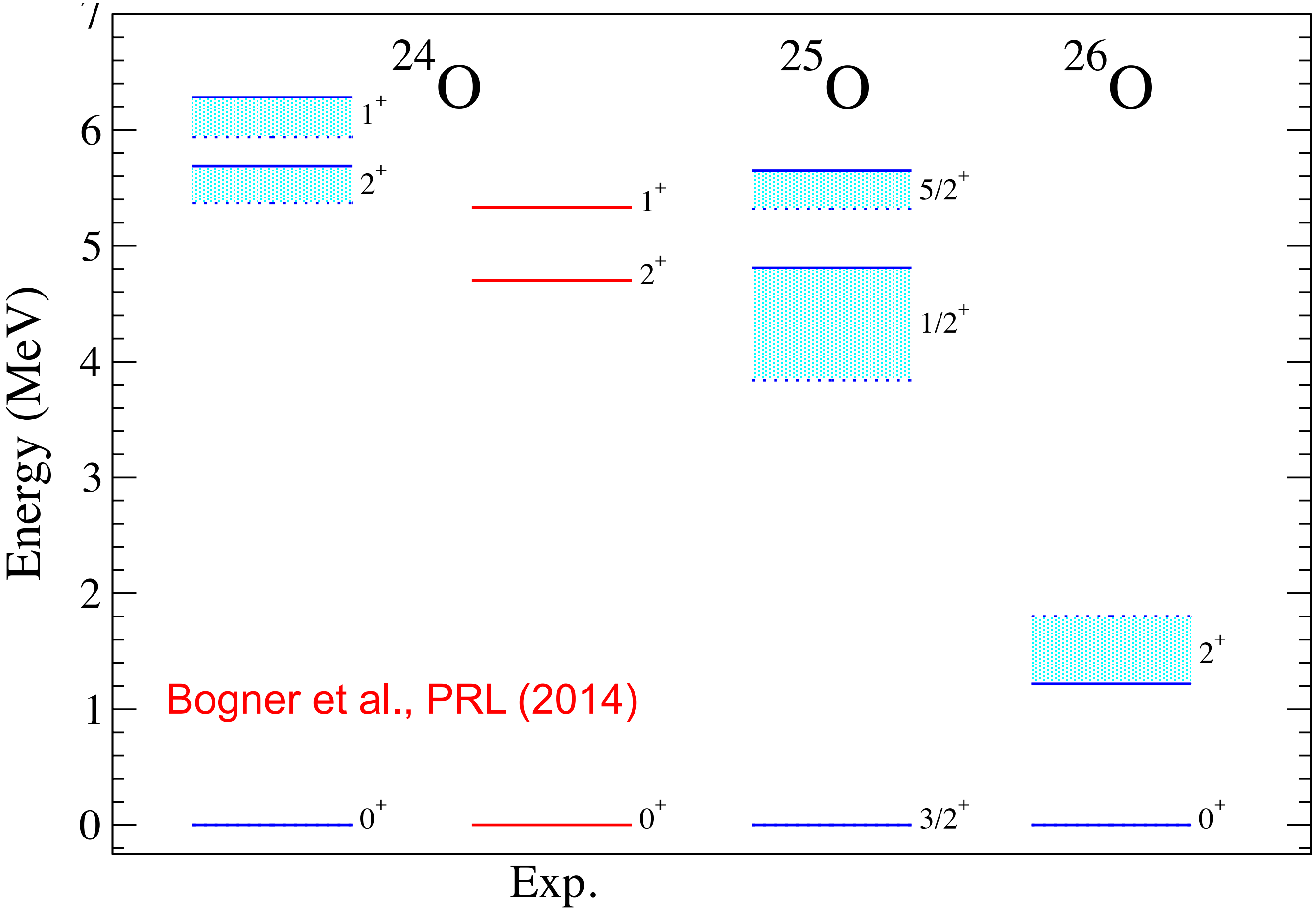


Clear improvement with NN+3N-full

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

IM-SRG Oxygen Spectra

Oxygen spectra: IM-SRG predictions beyond the dripline

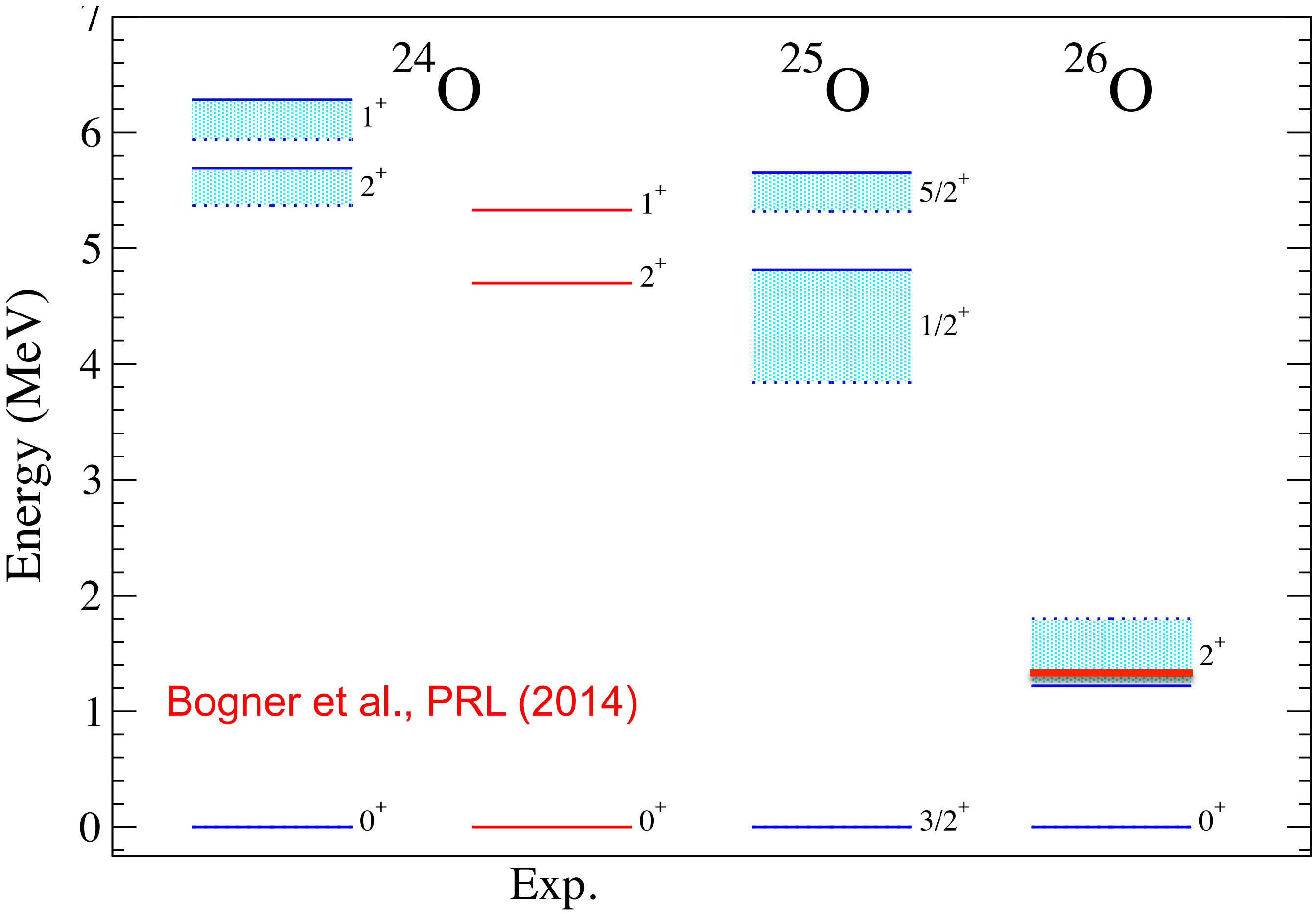


^{24}O closed shell (too high 2^+)

Continuum neglected: expect to lower spectrum

Experimental Connection: ^{26}O Spectrum

Oxygen spectra: IM-SRG predictions beyond the dripline



Kondo et al., PRELIMINARY

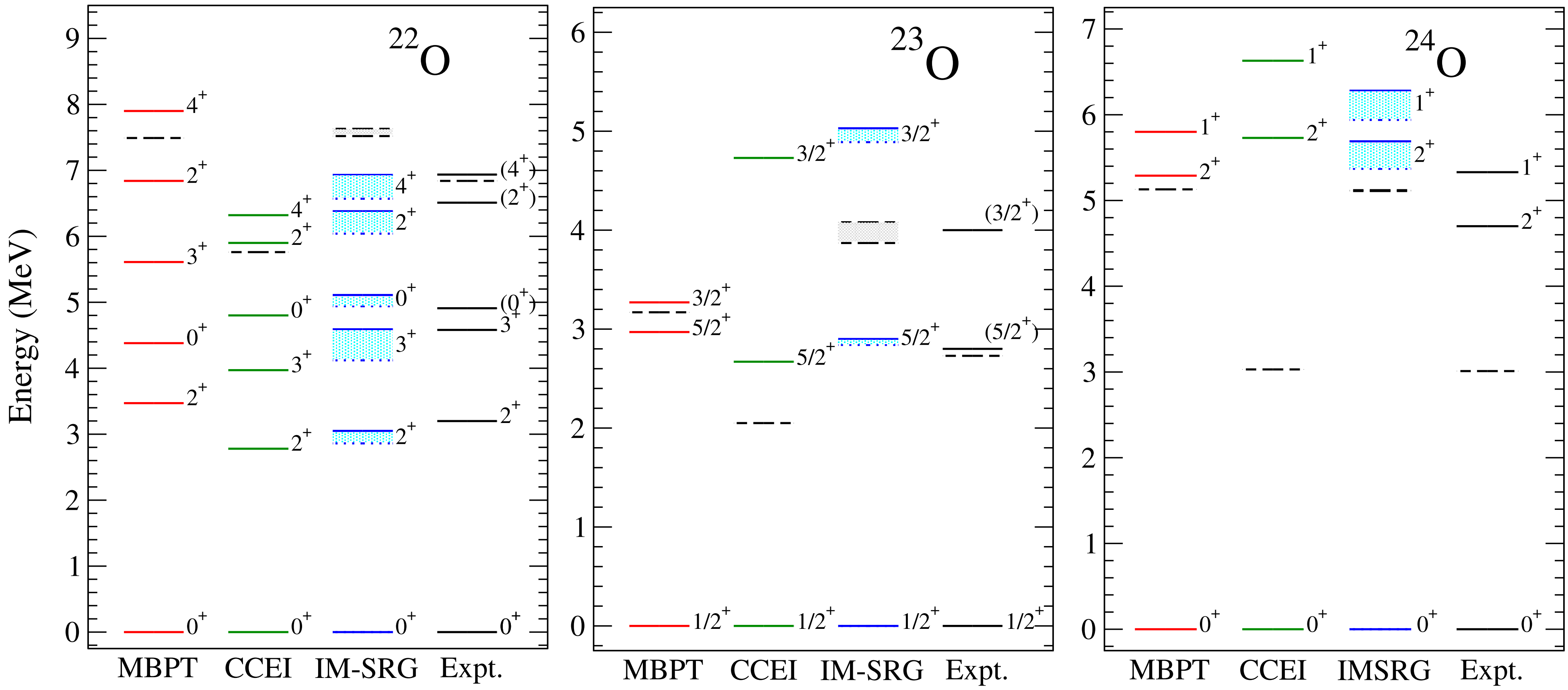
New measurement at RIKEN: excited states in ^{26}O

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**



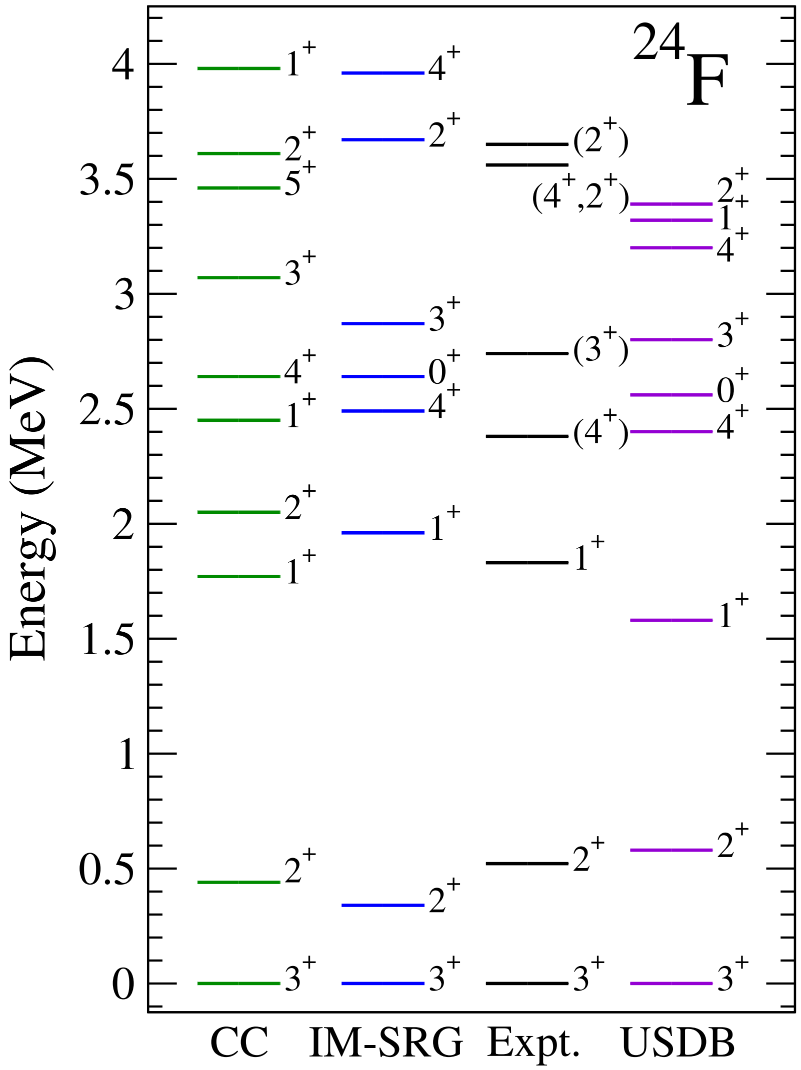
Hebeler, JDH, Menéndez, Schwenk, ARNPS (2015)

MBPT in extended valence space

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

Experimental Connection: ^{24}F Spectrum

^{24}F spectrum: **IM-SRG** (*sd* shell), **full CC**, **USDB**



Ekström et al., PRL (2014)

Cáceres et al., arXiv:1501.01166

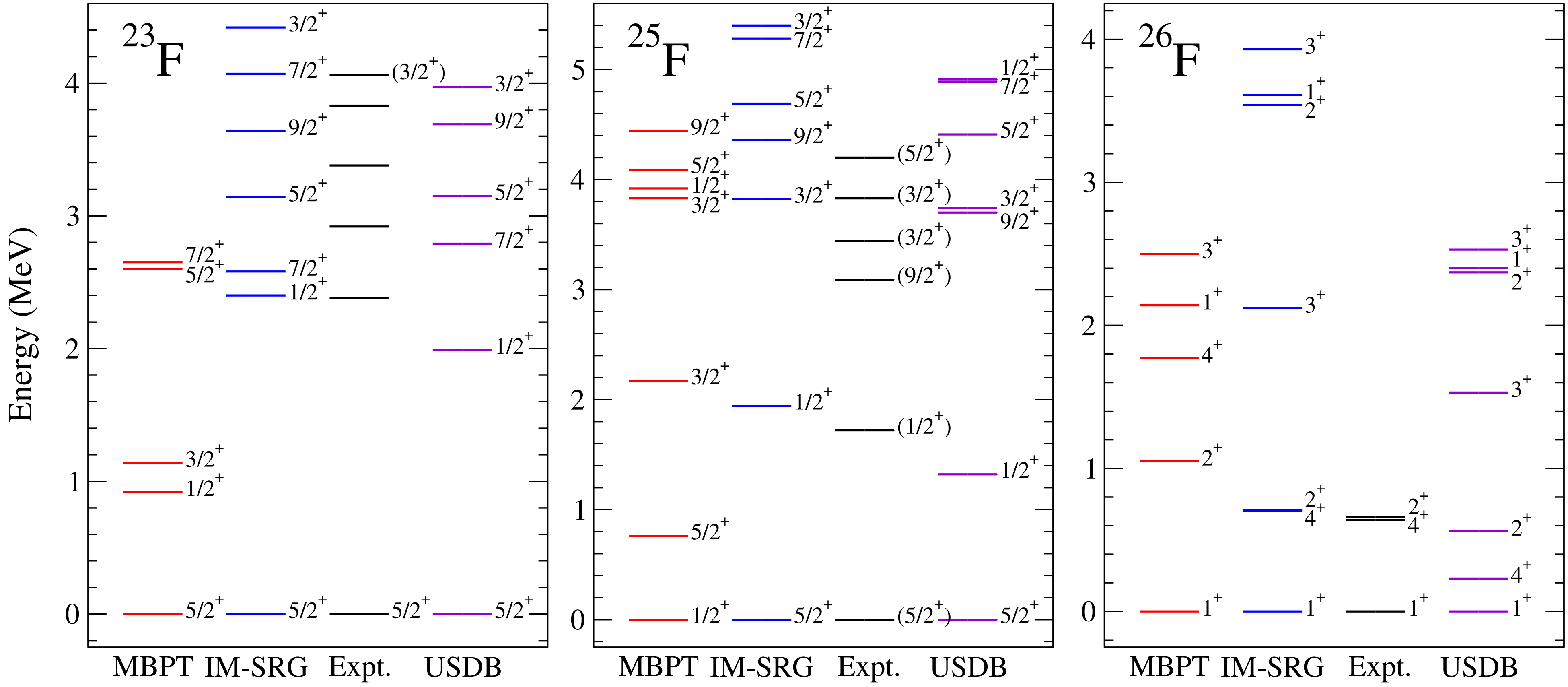
Hebeler, JDH, Menéndez, Schwenk, ARNPS (2015)

New measurements from GANIL

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

Fully Open Shell: Neutron-Rich Fluorine Spectra

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



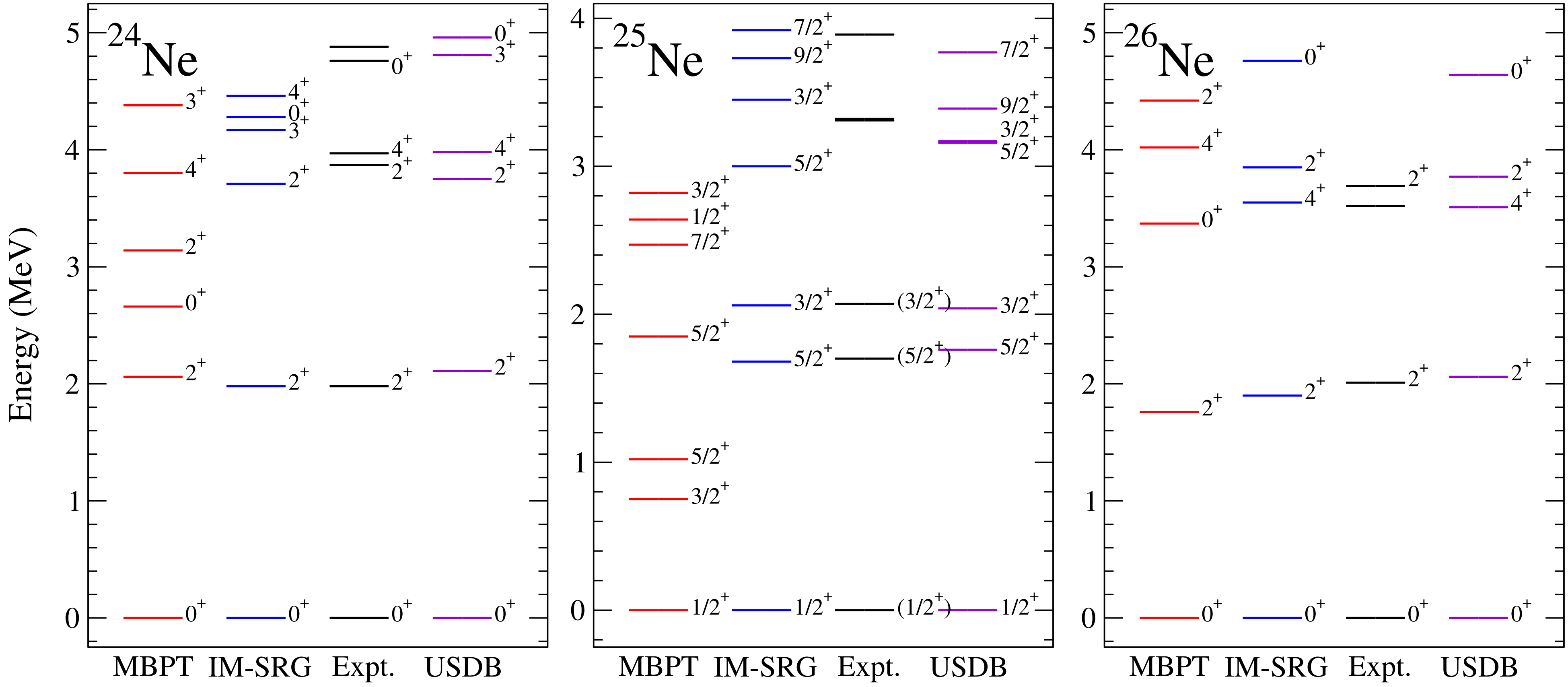
Bogner, Hergert, JDH, Schwenk, in prep.

MBPT: clear deficiencies

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)



Bogner, Hergert, JDH, Schwenk, in prep.

MBPT: clear deficiencies

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

Alternative Approach: Magnus Expansion

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

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

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

With flow equation:

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

Leads to commutator expression for evolved Hamiltonian

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

Nested commutator series – in practice truncate numerically

All calculations truncated at normal-ordered two-body level

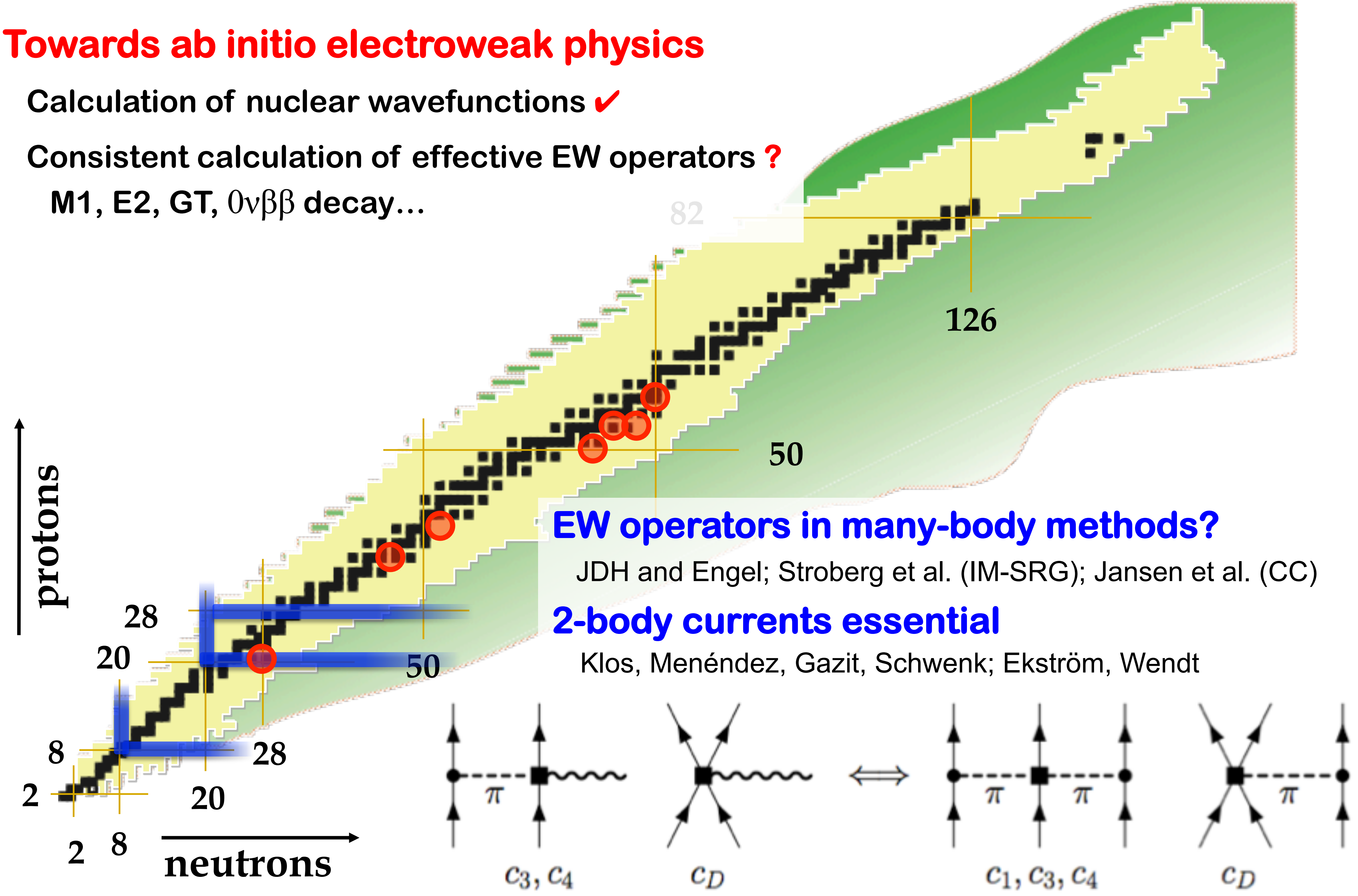
Prospect for Applications to Double-Beta Decay

Towards ab initio electroweak physics

Calculation of nuclear wavefunctions ✓

Consistent calculation of effective EW operators ?

M1, E2, GT, $0\nu\beta\beta$ decay…



EW operators in many-body methods?

JDH and Engel; Stroberg et al. (IM-SRG); Jansen et al. (CC)

2-body currents essential

Klos, Menéndez, Gazit, Schwenk; Ekström, Wendt

Improved 0νββ-Decay Calculations in Shell Model

Avenues towards ab initio shell model calculations

Consistent operators and wavefunctions

$$M^{0\nu} = M^{0\nu}_{GT} - \frac{M^{0\nu}_{F}}{g_A^2} + M^{0\nu}_{T}$$

$$M^{0\nu}_{GT} = \langle f | \underbrace{\sum_{ab} H(r_{ab})\vec{\sigma}_a \cdot \vec{\sigma}_b \tau^+_a \tau^+_b}_{\mathbf{M_{eff}}} | i \rangle$$

$$M^{0\nu}_{F} = \langle f | \underbrace{\sum_{ab} H(r_{ab})\tau^+_a \tau^+_b}_{\mathbf{M_{eff}}} | i \rangle$$

1) Nuclear wavefunctions: currently phenomenological – calculate ab initio

2) **Effective decay operator**: **correlations outside valence space**

E0 Transitions and Radii

Seldom calculated in nuclear shell model

In single HO shell:

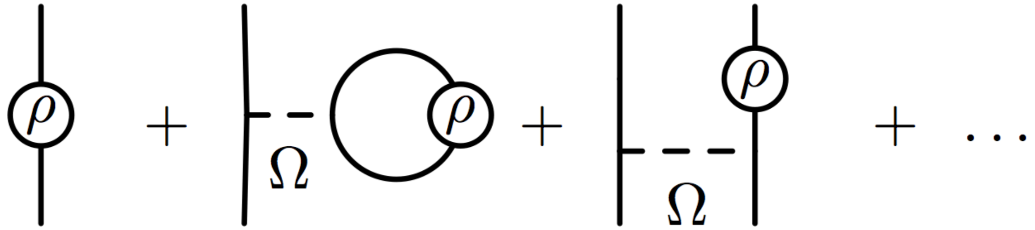
$$|\langle f|\rho_{E0}|i\rangle|^2 \propto \delta_{ij} \text{ where } \rho_{E0} = \frac{1}{e^2 R}\sum_i e_i r_i^2$$

Must resort to phenomenological gymnastics

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!

Drip Lines and Magic Numbers: The Nuclear Landscape Toward the Extremes

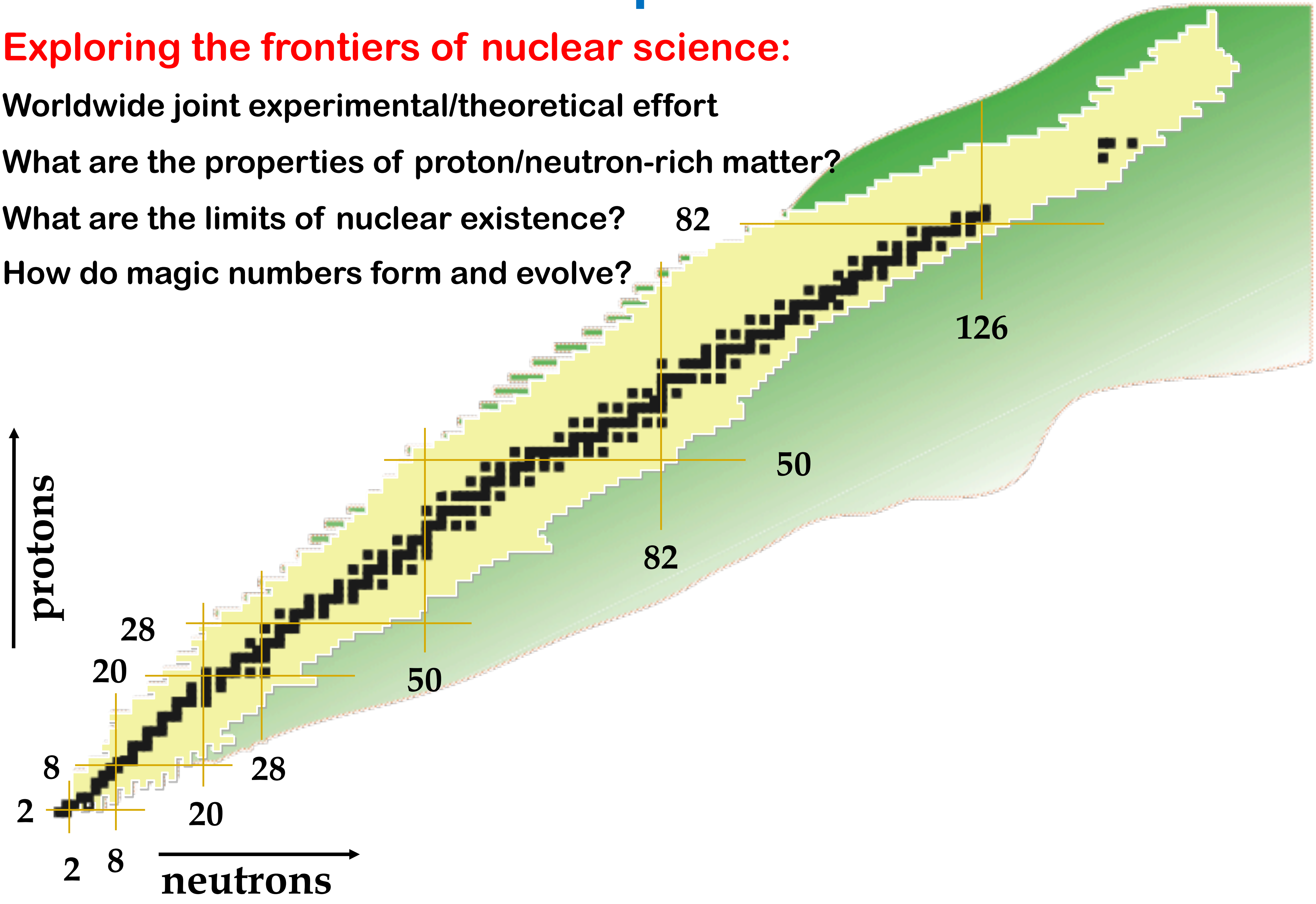
Exploring the frontiers of nuclear science:

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?



Advances in ab initio Nuclear Structure for Medium-Mass Exotic Nuclei

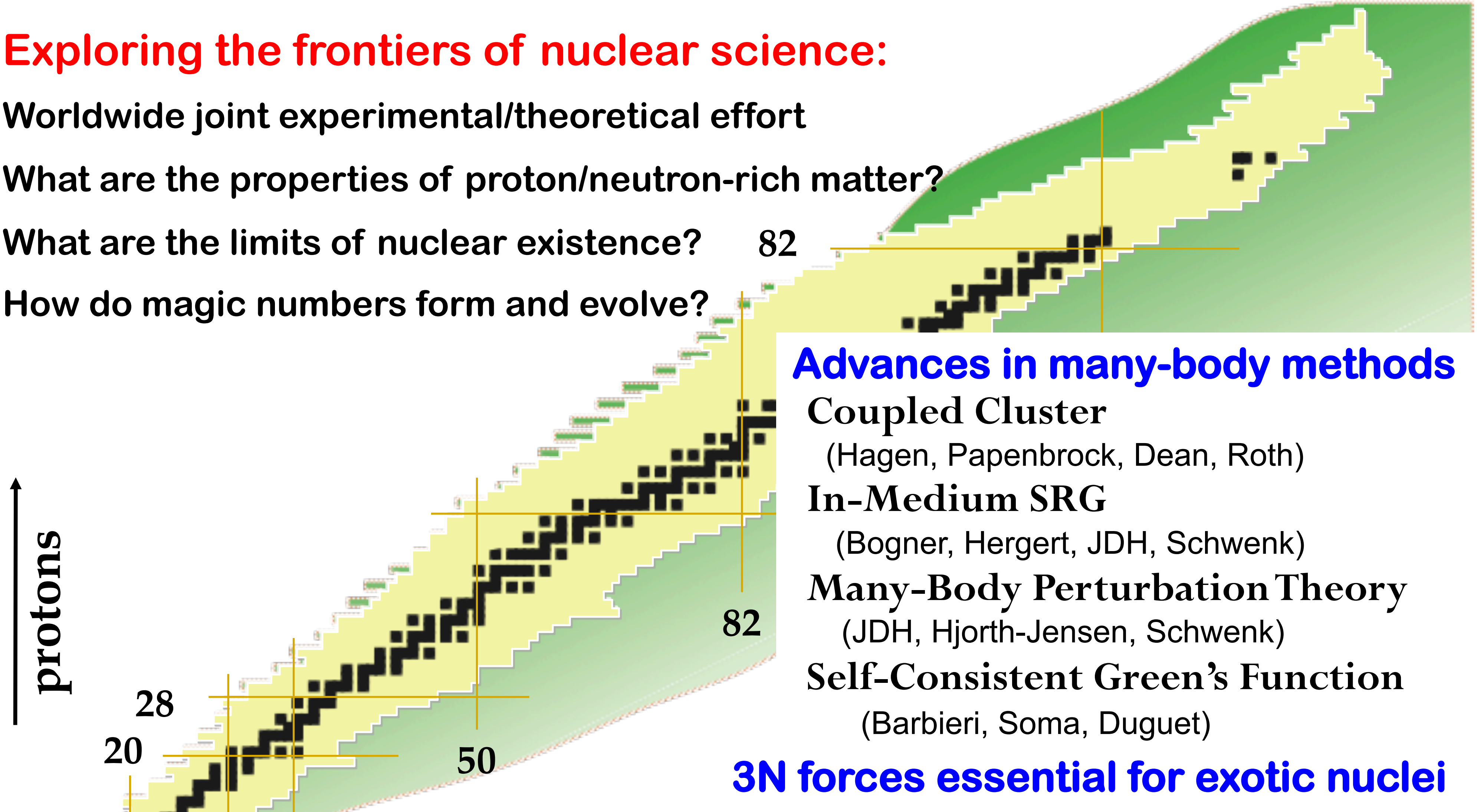
Exploring the frontiers of nuclear science:

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?



Advances in many-body methods

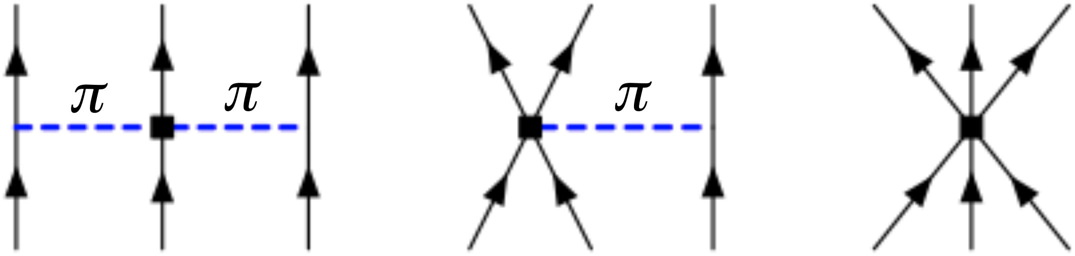
Coupled Cluster
(Hagen, Papenbrock, Dean, Roth)

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

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

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

3N forces essential for exotic nuclei



Advances in ab initio Nuclear Structure for Medium-Mass Exotic Nuclei

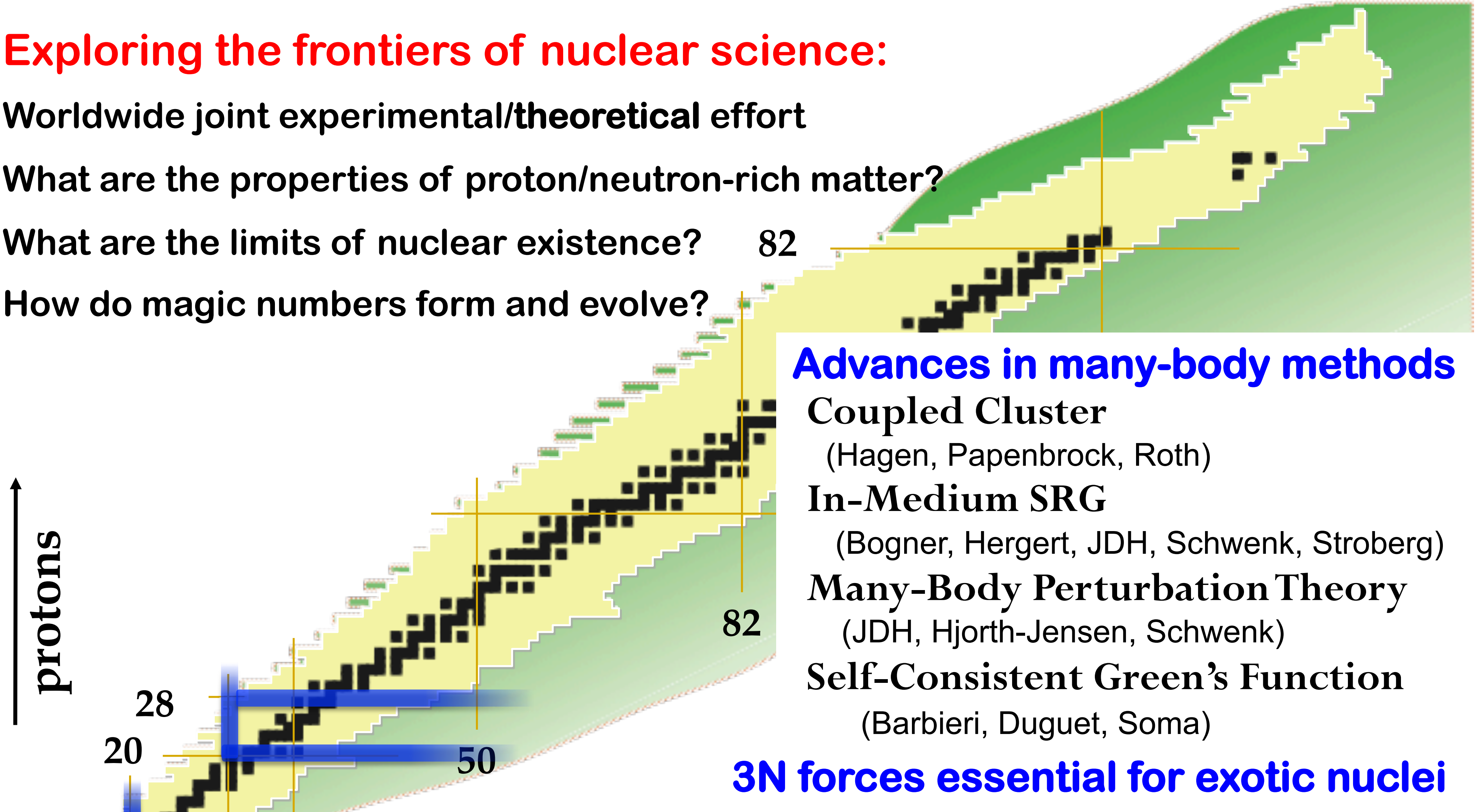
Exploring the frontiers of nuclear science:

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?



Advances in many-body methods

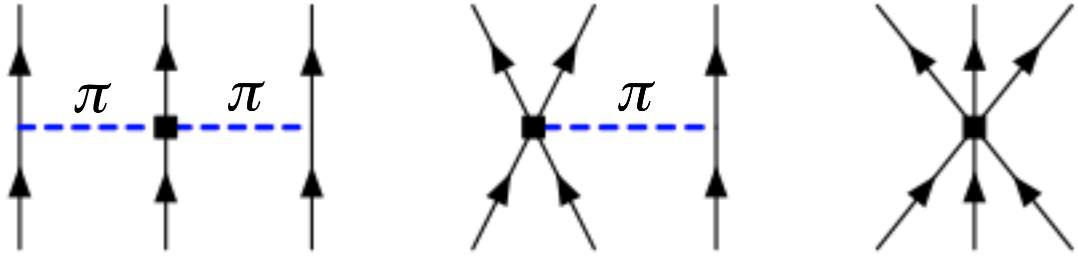
Coupled Cluster
(Hagen, Papenbrock, Roth)

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

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

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

3N forces essential for exotic nuclei



Advances in ab initio Nuclear Structure for Medium-Mass Exotic Nuclei

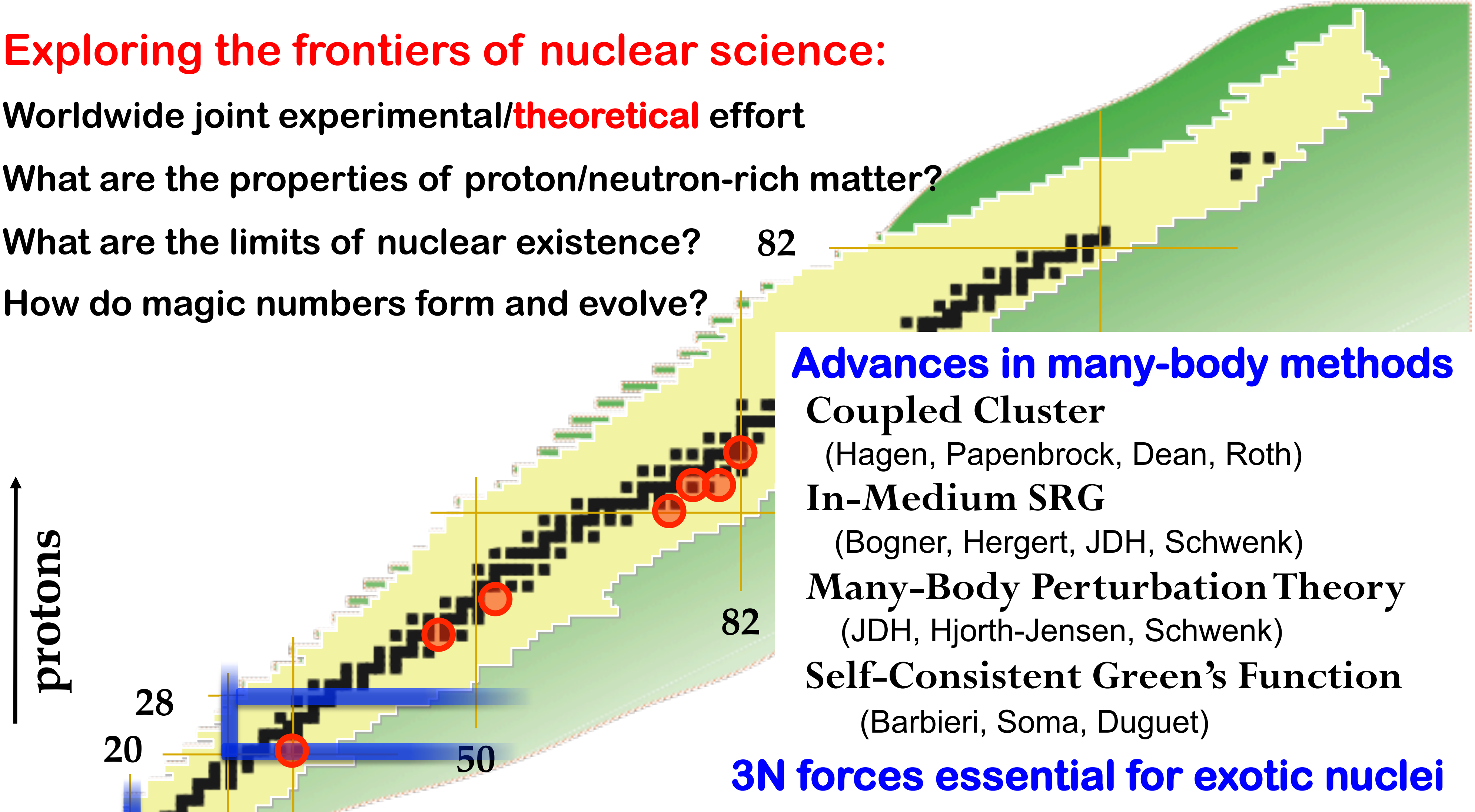
Exploring the frontiers of nuclear science:

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?



Advances in many-body methods

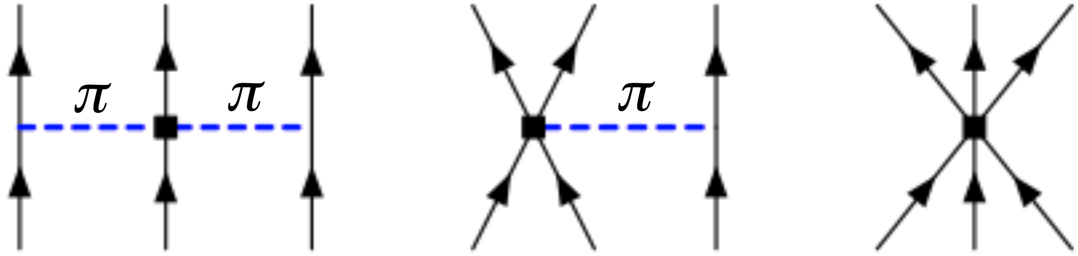
Coupled Cluster
(Hagen, Papenbrock, Dean, Roth)

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

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

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

3N forces essential for exotic nuclei

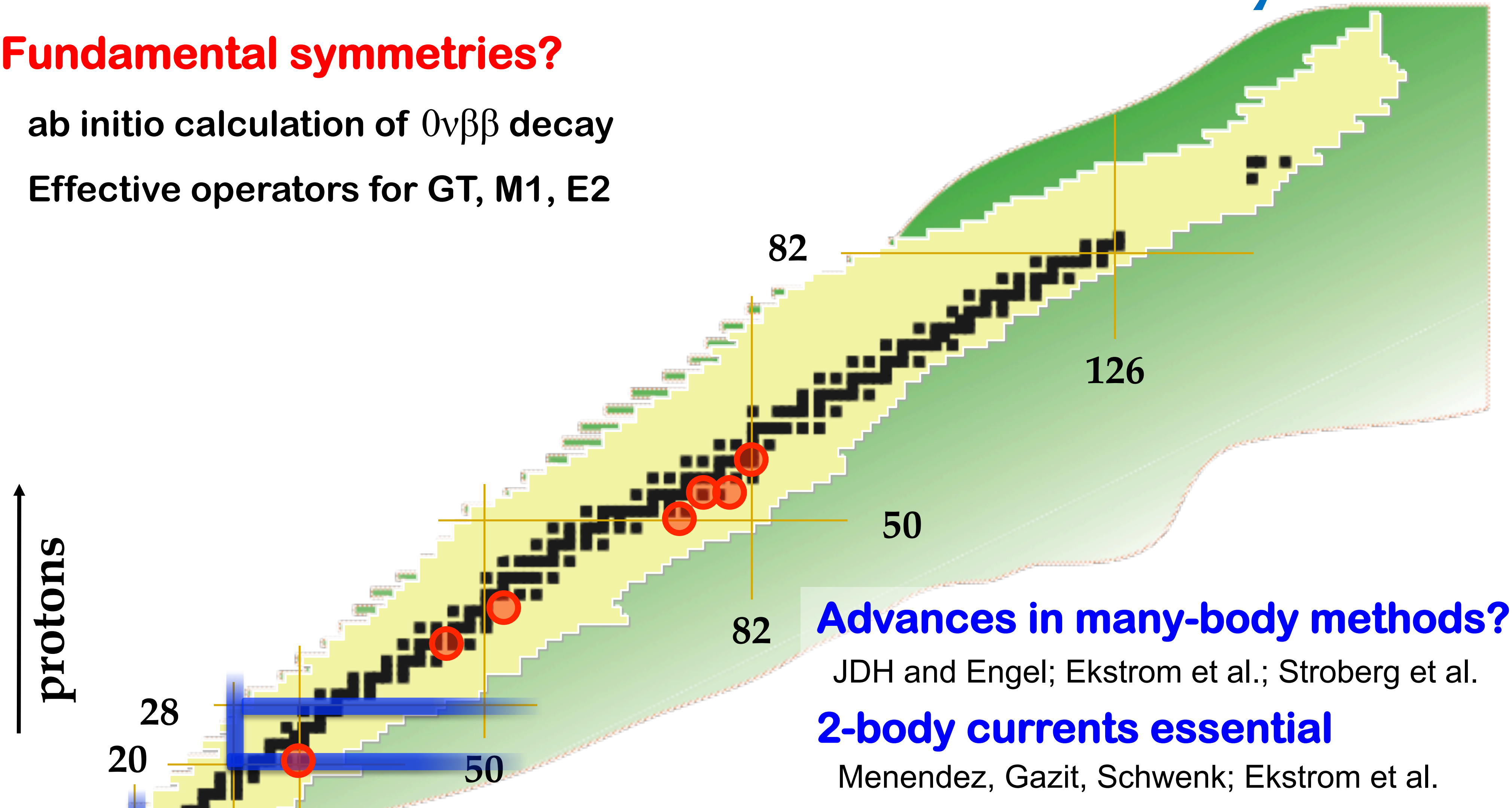


Prospect for Applications to Neutrinoless Double-Beta Decay

Fundamental symmetries?

ab initio calculation of $0\nu\beta\beta$ decay

Effective operators for GT, M1, E2

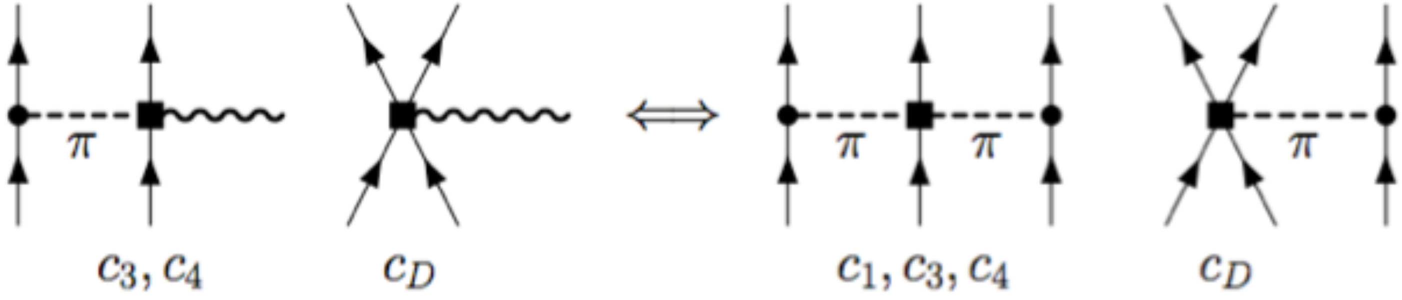


Advances in many-body methods?

JDH and Engel; Ekstrom et al.; Stroberg et al.

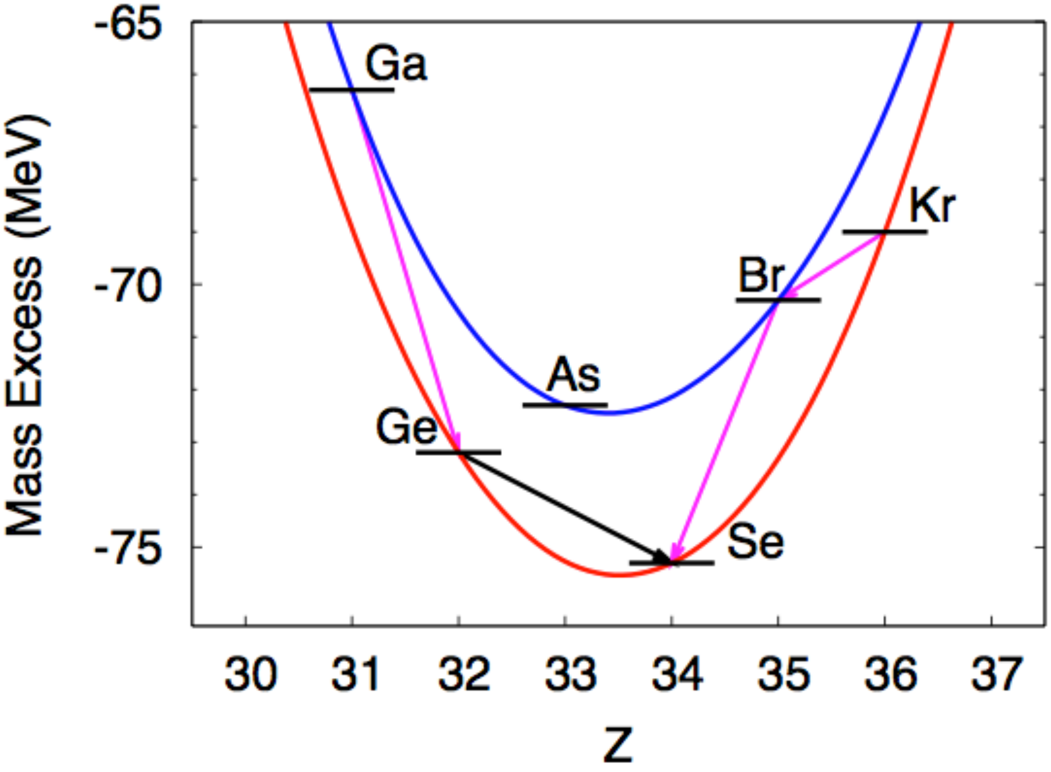
2-body currents essential

Menendez, Gazit, Schwenk; Ekstrom et al.



Nuclear Weak Processes: ββ-Decay

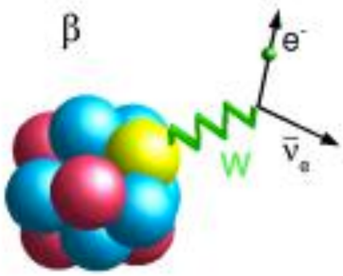
Nuclear weak processes: fundamental importance for particle physics

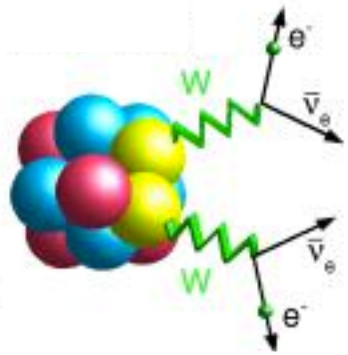


Rare cases when single β-decay
is energetically forbidden

Can undergo ββ-decay

Second-order weak process



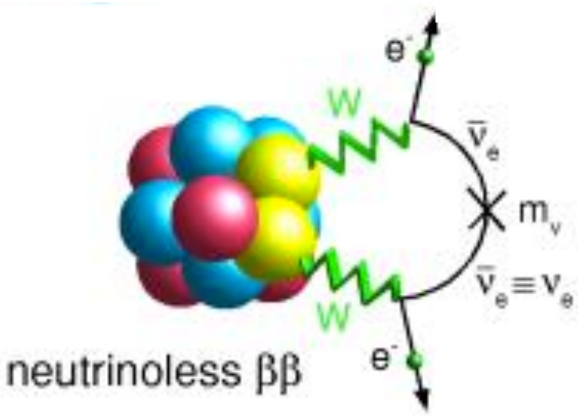


Observed in 15 nuclei with:

$$(T_{1/2}^{2\nu\beta\beta})^{-1} \approx 10^{19}\,\mathrm{y}$$

Fundamental Symmetries: 0νββ-Decay

Assuming exchange of light neutrinos



Two essential ingredients:

Q-value (experiment)

Nuclear matrix element

$$(T_{1/2}^{0\nu\beta\beta})^{-1} = G^{0\nu}(Q_{\beta\beta}, Z)\left|M^{0\nu}\right|^2\left(\frac{\langle m_{\beta\beta}\rangle}{m_e}\right)^2 \qquad \langle m_{\beta\beta}\rangle = \left|\sum_{i=1}^{3} U_{ei} m_i\right|$$

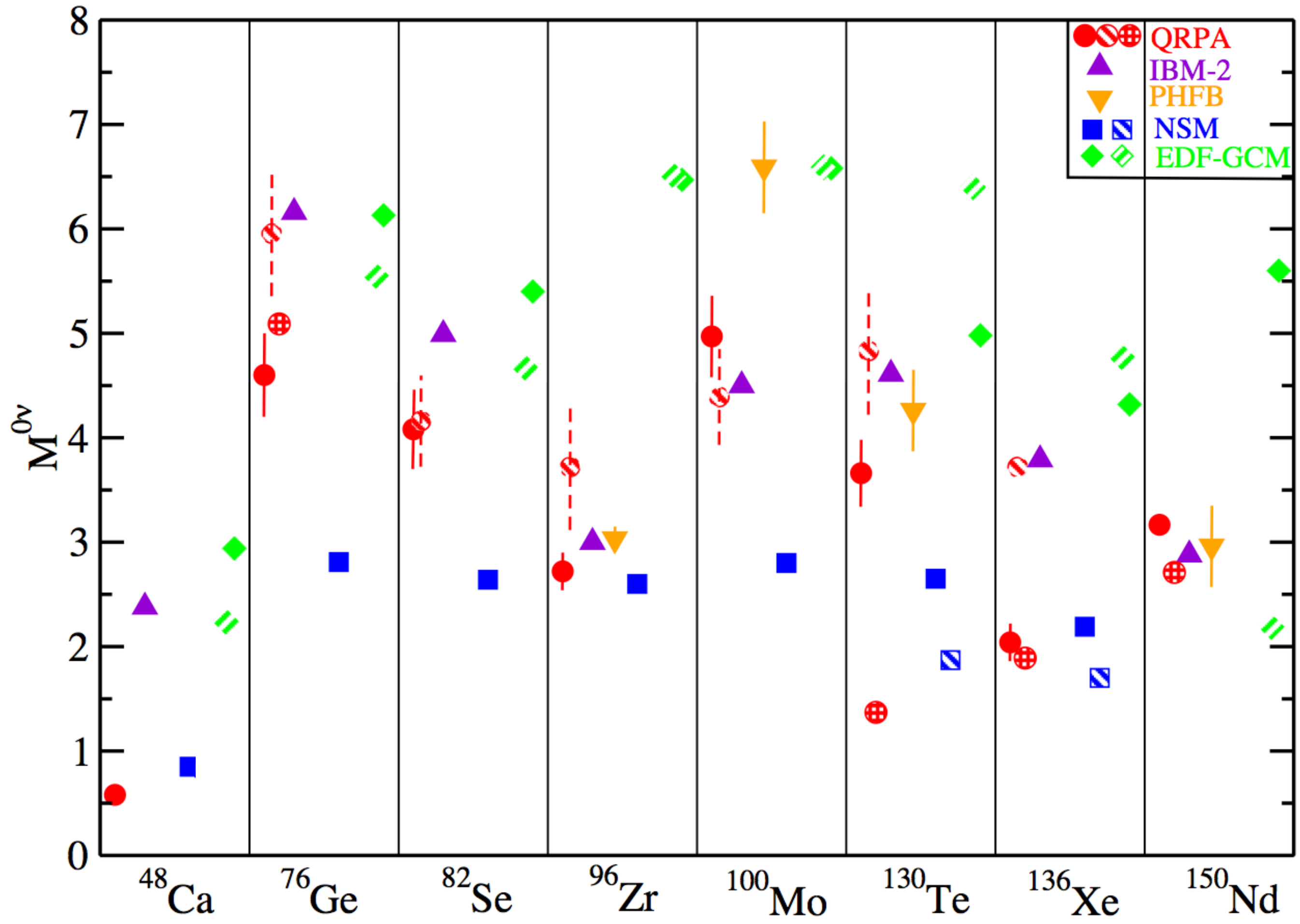
Character of neutrino (Majorana/Dirac)

Lepton number violation

Neutrino mass scale

Nuclear Matrix Element

Recent calculations of NME: pronounced differences for lighter candidates



Shell model: exact correlations in truncated single-particle space

QRPA, EDF, IBM: schematic correlations in large single-particle space

Aim: first-principles framework capable of robust prediction

Improved 0νββ-Decay Calculations in Shell Model

Avenues towards ab initio shell model calculations

Consistent operators and wavefunctions

$$M^{0\nu} = M^{0\nu}_{GT} - \frac{M^{0\nu}_{F}}{g_A^2} + M^{0\nu}_{T}$$

$$M^{0\nu}_{GT} = \langle f | \sum_{ab} H(r_{ab}) \vec{\sigma}_a \cdot \vec{\sigma}_b \tau_a^+ \tau_b^+ | i \rangle$$

$$M^{0\nu}_{F} = \langle f | \sum_{ab} H(r_{ab}) \tau_a^+ \tau_b^+ | i \rangle$$

1) **Nuclear wavefunctions**: currently phenomenological – calculate ab initio

Effective 0νββ-Decay Operator

Calculate in MBPT:

1st order (× 2)

Improved 0νββ-Decay Calculations in Shell Model

Avenues towards ab initio shell model calculations

Consistent operators and wavefunctions

$$M^{0\nu} = M_{GT}^{0\nu} - \frac{M_{F}^{0\nu}}{g_A^2} + M_{T}^{0\nu}$$

$$M_{GT}^{0\nu} = \langle f | \underbrace{\sum_{ab} H(r_{ab}) \vec{\sigma}_a \cdot \vec{\sigma}_b \tau_a^+ \tau_b^+}_{\mathbf{M}_{\mathbf{eff}}} | i \rangle$$

$$M_{F}^{0\nu} = \langle f | \underbrace{\sum_{ab} H(r_{ab}) \tau_a^+ \tau_b^+}_{\mathbf{M}_{\mathbf{eff}}} | i \rangle$$

1) Nuclear wavefunctions: currently phenomenological – calculate ab initio
2) **Effective decay operator**: **correlations outside valence space**

Improved 0νββ-Decay Calculations in Shell Model

Avenues towards ab initio shell model calculations

Consistent operators and wavefunctions

$$M^{0\nu} = M^{0\nu}_{GT} - \frac{M^{0\nu}_F}{g_A^2} + M^{0\nu}_T$$

$$M^{0\nu}_{GT} = \langle f | \sum_{ab} H(r_{ab}) \vec{\sigma}_a \cdot \vec{\sigma}_b \tau^+_a \tau^+_b | i \rangle$$

$$M^{0\nu}_F = \langle f | \sum_{ab} H(r_{ab}) \tau^+_a \tau^+_b | i \rangle$$

1) Nuclear wavefunctions: currently phenomenological – calculate ab initio
2) Effective decay operator: correlations outside valence space
3) Improvements in operator: two-body currents

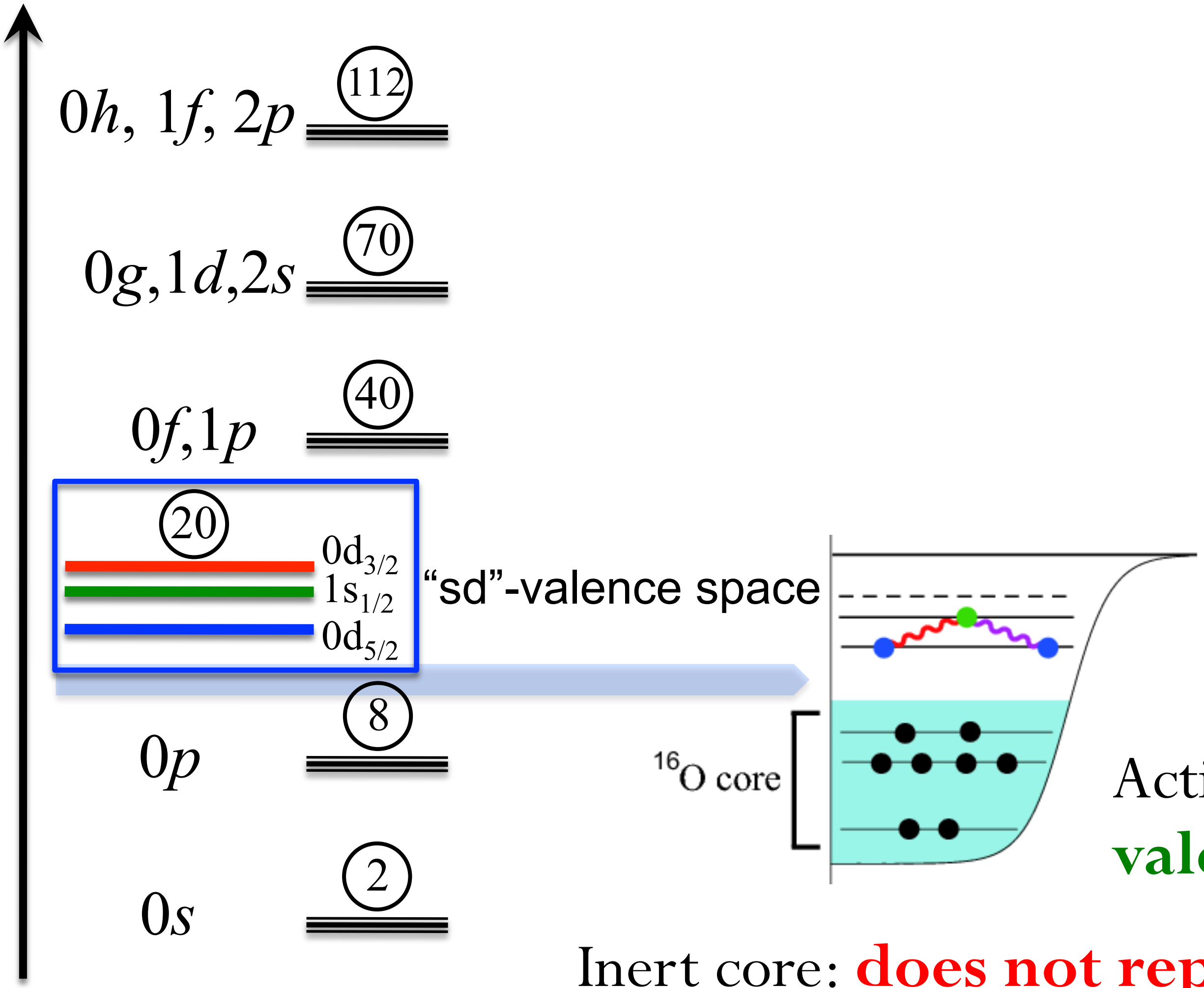
The Nuclear Many-Body Problem

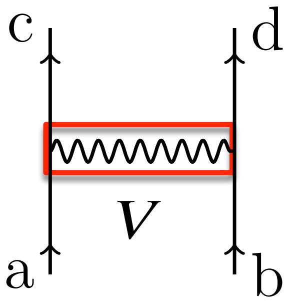
Nuclei understood as many-body system starting from closed shell, add nucleons

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**

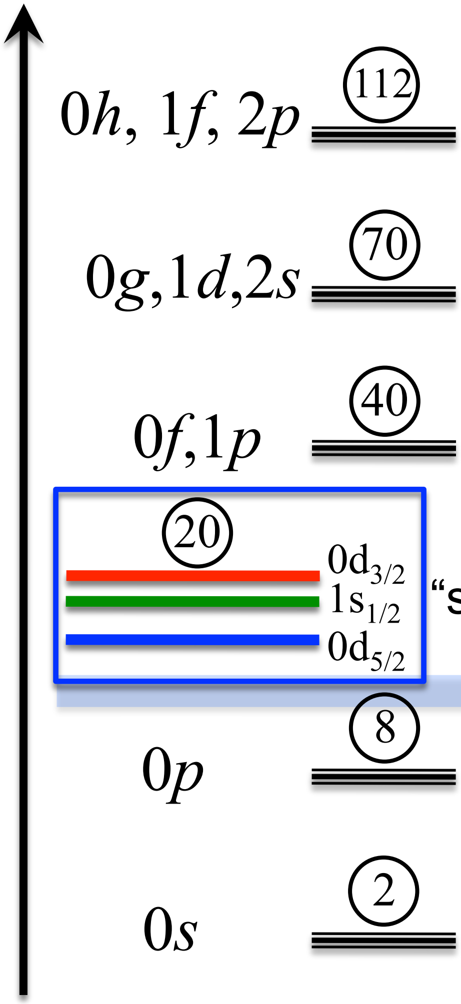
The Nuclear Many-Body Problem

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

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

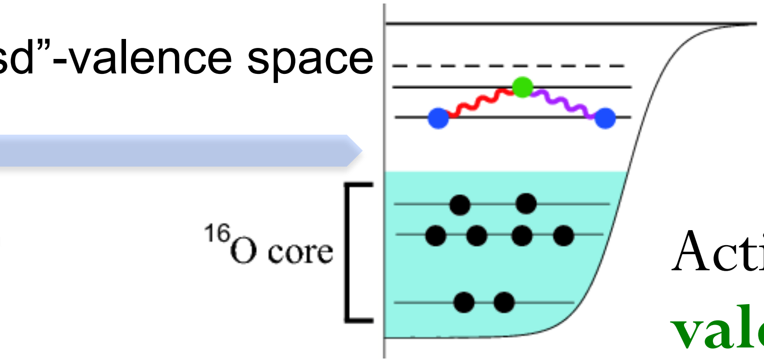
Interaction matrix elements

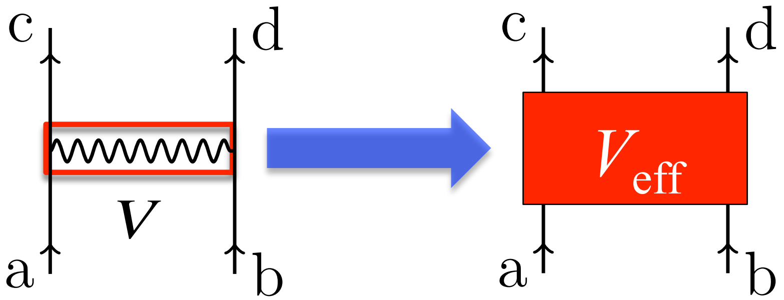
Single-particle energies (SPEs)



Solution: allow breaking of core

Effective Hamiltonian for valence nucleons



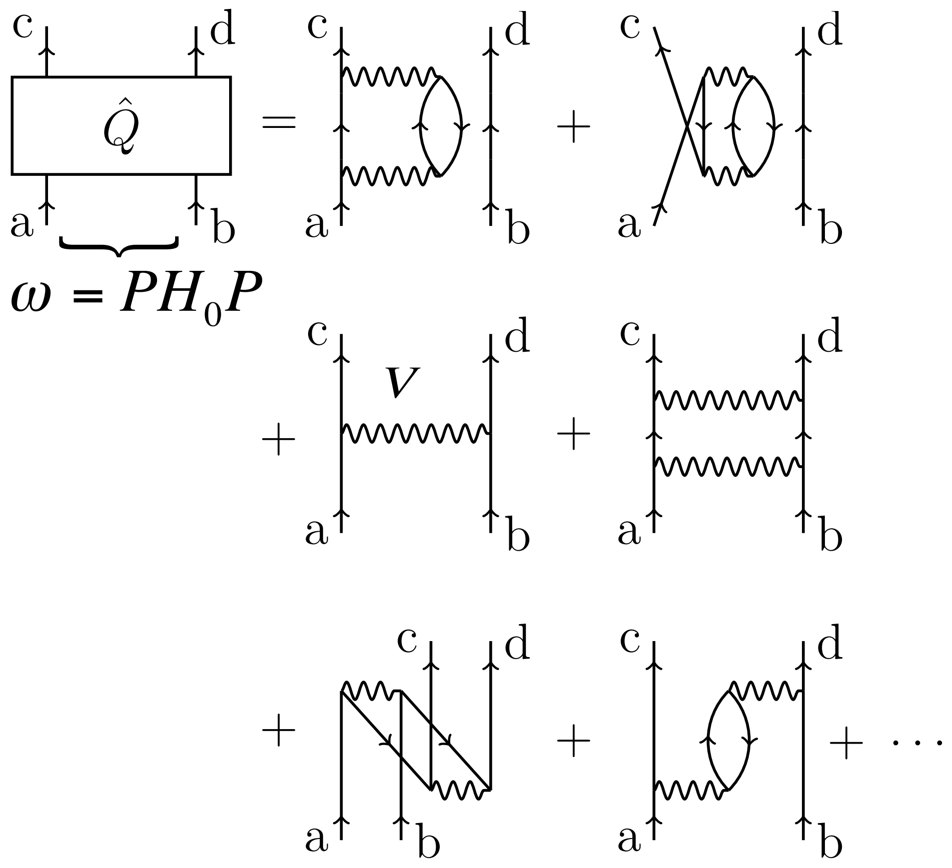


Active nucleons occupy **valence space**

Many-Body Perturbation Theory

First calculate **energy dependent** effective interaction

$$\hat{Q}(\omega) = PVP + PVQ\boxed{\frac{1}{\omega - QHQ}}QVP$$



$\omega = PH_0P$

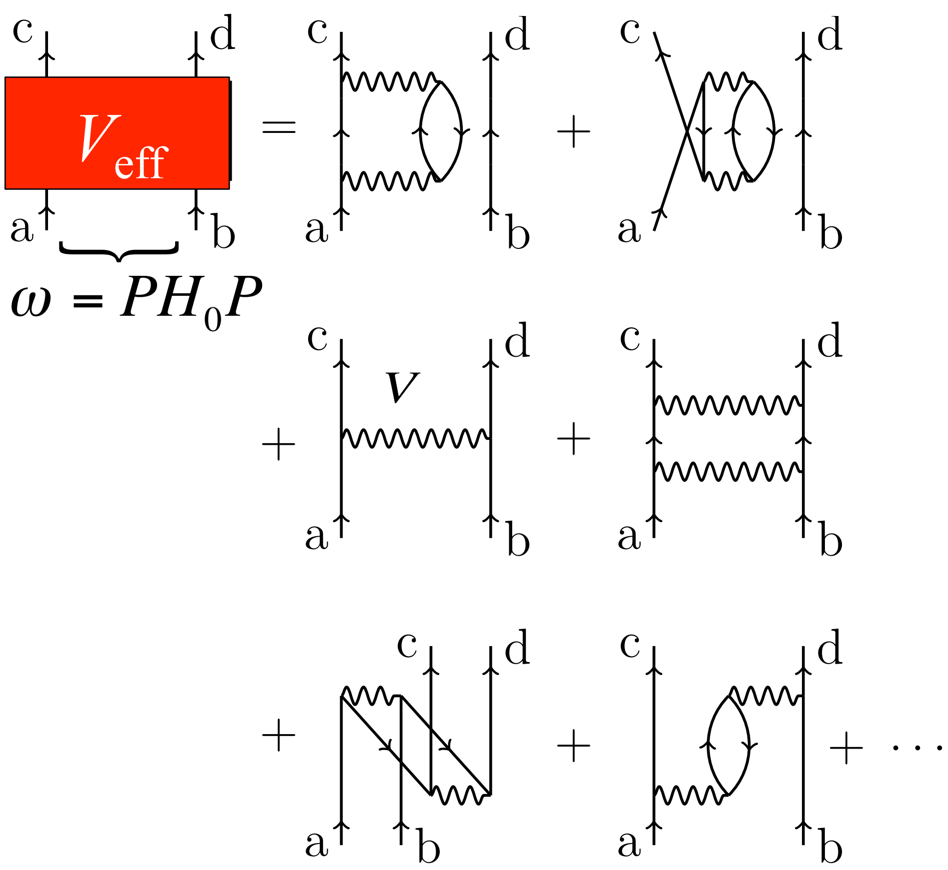
Effects of excitations outside valence space

Approximation: sum $\hat{Q}(\omega)$ to finite order

Many-Body Perturbation Theory

First calculate **energy dependent** effective interaction

$$\hat{Q}(\omega) = PVP + PV\boxed{Q\frac{1}{\omega - QHQ}Q}VP$$



$$\omega = PH_0P$$

Effects of excitations outside valence space

Approximation: sum $\hat{Q}(\omega)$ to finite order

Nonperturbative folded diagrams
to remove energy dependence

$$V_{\text{eff}}^{(n)} = \hat{Q} + \sum_{m=1}^{\infty} \frac{1}{m!} \frac{\mathrm{d}^m \hat{Q}}{\mathrm{d}\omega^m} \left\{ V_{\text{eff}}^{(n-1)} \right\}^m$$

Eigenvalues converge to exact values of A-body Hamiltonian with largest model-space overlap

Perturbative Valence-Space Strategy

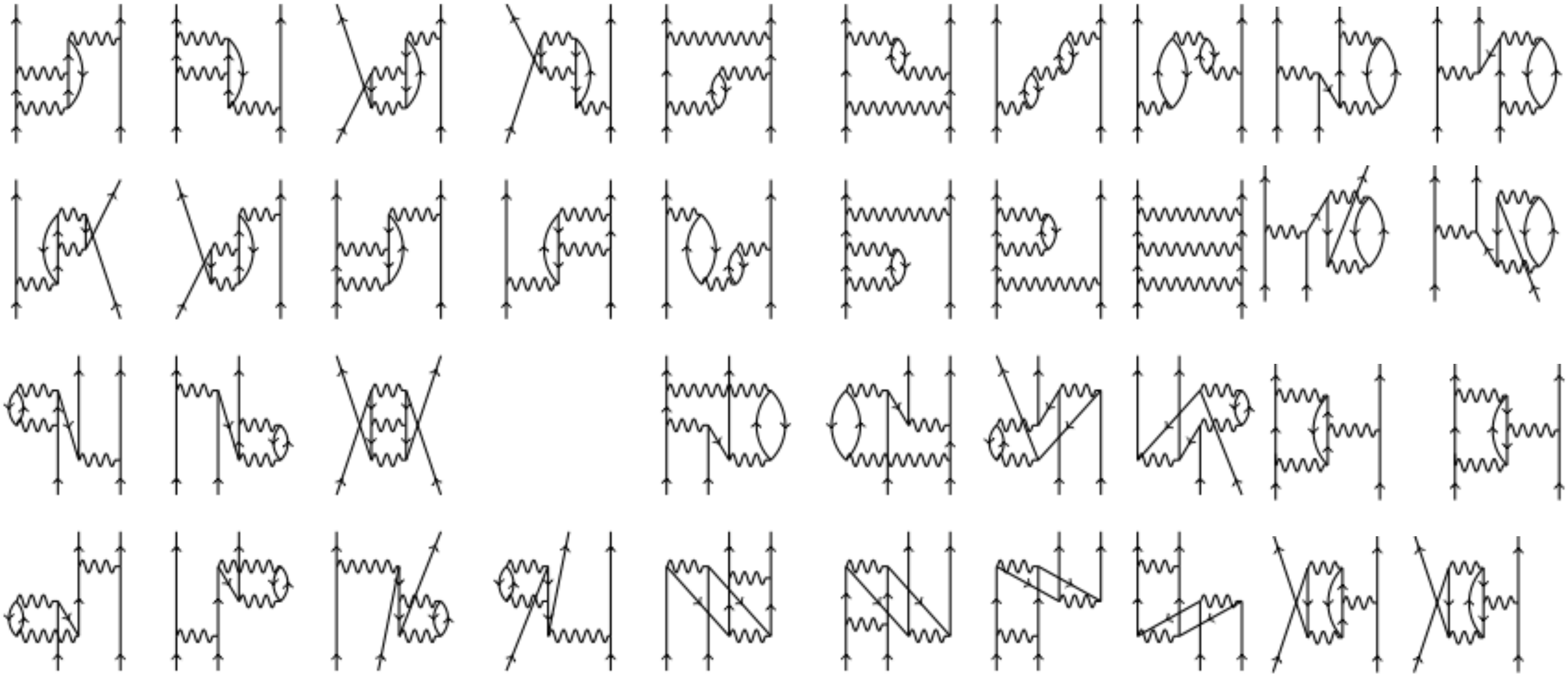
★1) Effective interaction: sum excitations outside valence space to **3rd order**

★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 3rd-order MBPT

5) Explore extended valence spaces



Perturbative Valence-Space Strategy

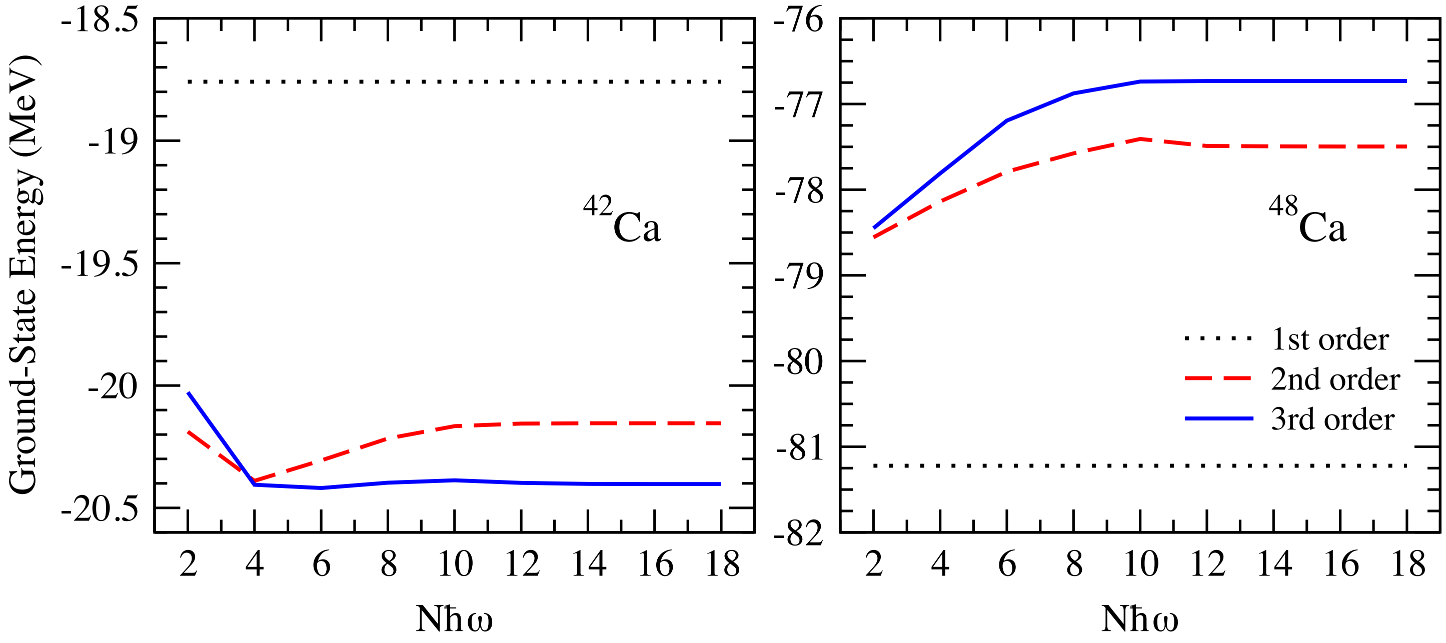
1) Effective interaction: sum excitations outside valence space to **3rd order**

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 3rd-order MBPT

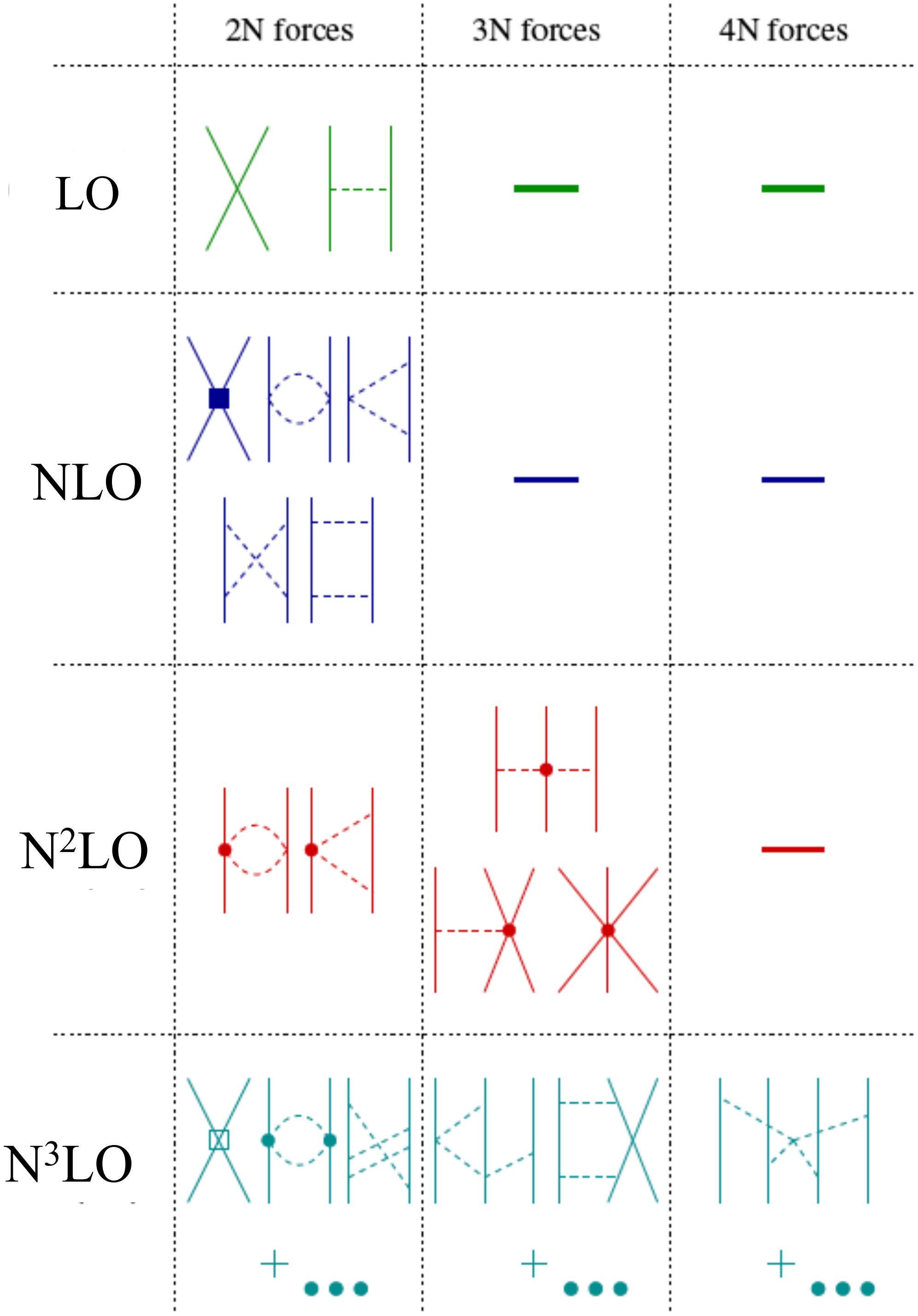
5) Explore extended valence spaces



Clear convergence with HO basis size

Promising order-by-order behavior – compare with ab initio methods

Chiral Effective Field Theory: Nuclear Forces



Nucleons interact via pion exchanges and contact interactions

Consistent treatment of NN, 3N,… 2-body currents

3N couplings fit to properties of light nuclei at low momentum

Improve convergence of many-body methods:

$$V_{\text{low }k} \quad \text{or} \quad V_{\text{SRG}}$$

Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Meissner,…

Perturbative Valence-Space Strategy

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

5) Explore extended valence spaces

NN matrix elements

- Chiral N^3LO (Machleidt, $\Lambda_{NN} = 500\text{MeV}$); smooth-regulator $V_{\text{low }k}(\Lambda)$

3N force contributions

- Chiral N^2LO
  c_D, c_E fit to properties of light nuclei with $V_{\text{low }k}$ $(\Lambda = \Lambda_{3N} = 2.0\text{fm}^{-1})$
- Included to 5 major HO shells

Perturbative Valence-Space Strategy

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

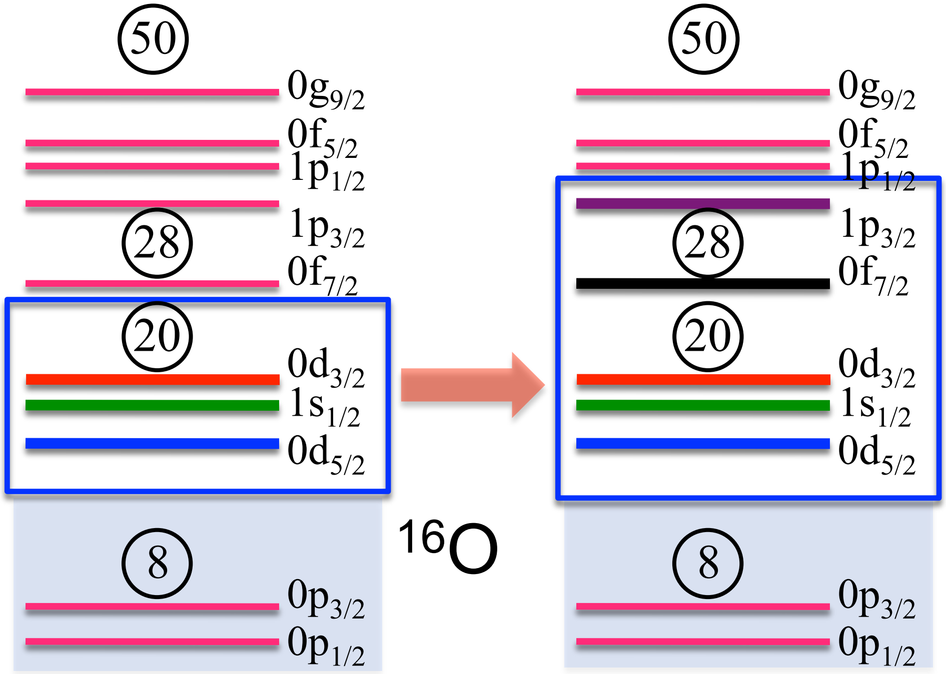
2) Single-particle energies calculated self consistently

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

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

★ 5) Explore **extended valence spaces**

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



Treats higher orbits nonperturbatively

When important for exotic nuclei?

Best option for double-beta decay?

Nuclear Wavefunctions: Calcium Isotopes

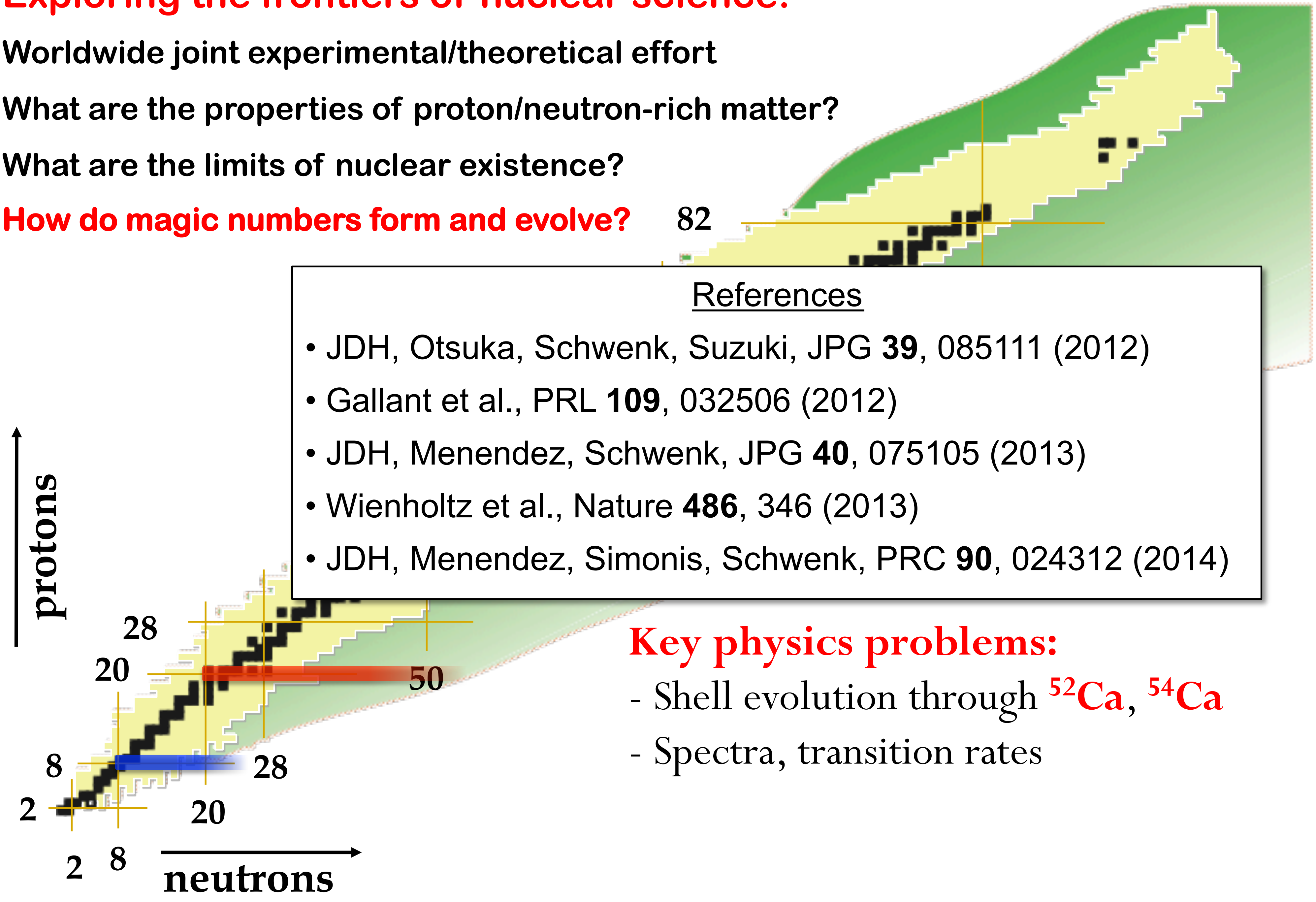
Exploring the frontiers of nuclear science:

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?



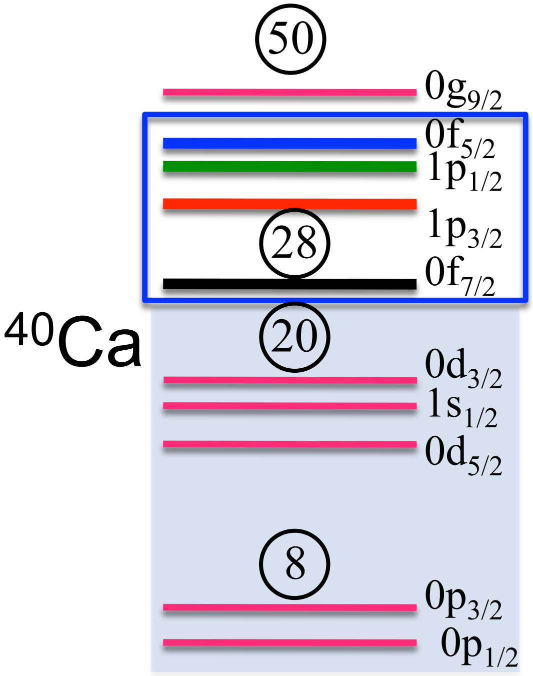
References

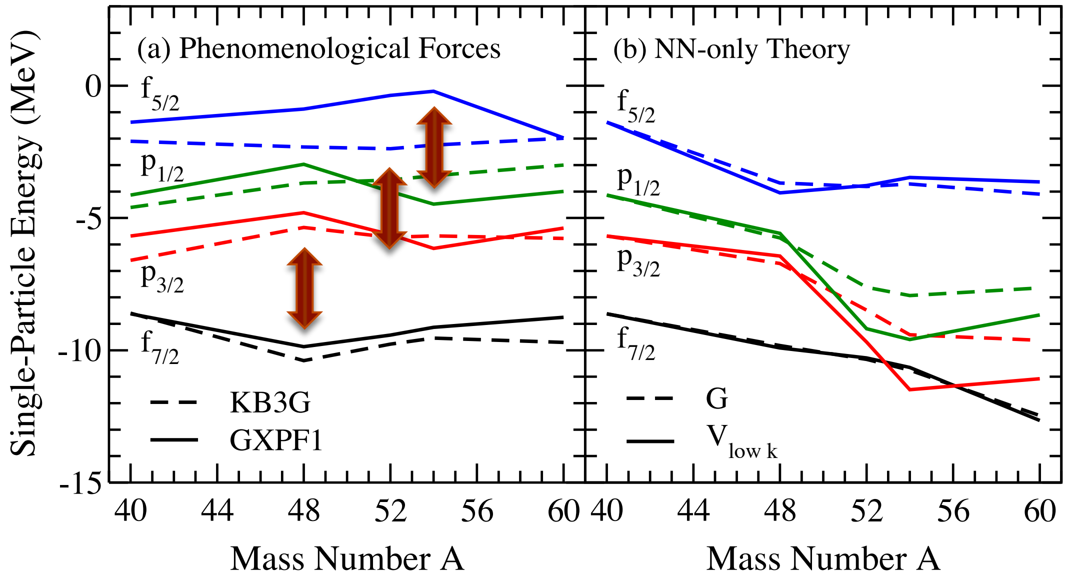
- JDH, Otsuka, Schwenk, Suzuki, JPG **39**, 085111 (2012)
- Gallant et al., PRL **109**, 032506 (2012)
- JDH, Menendez, Schwenk, JPG **40**, 075105 (2013)
- Wienholtz et al., Nature **486**, 346 (2013)
- JDH, Menendez, Simonis, Schwenk, PRC **90**, 024312 (2014)

Key physics problems:

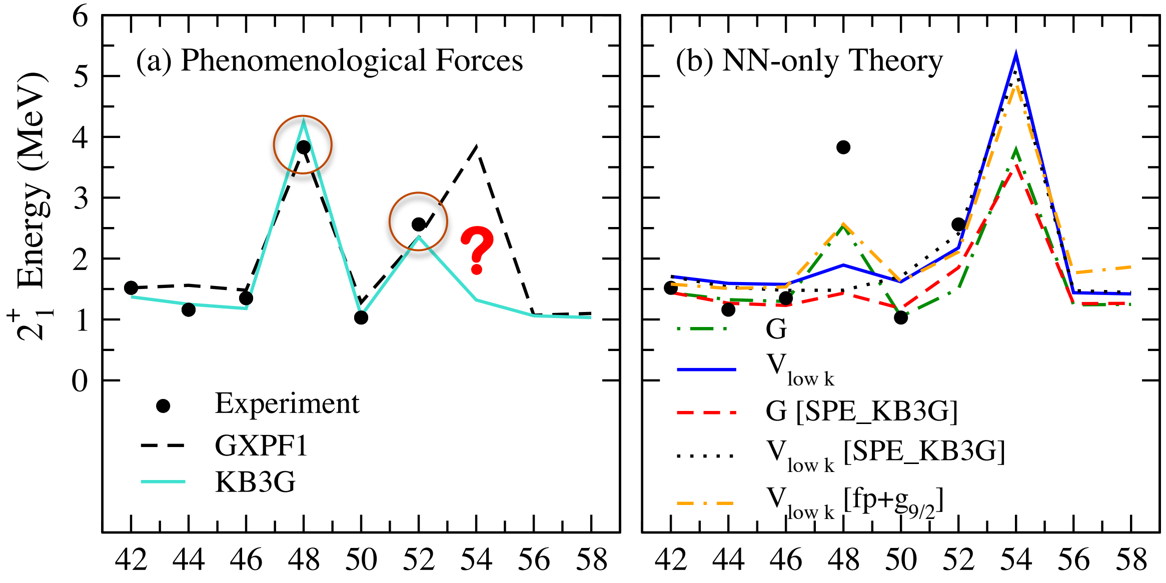
- Shell evolution through ^{52}Ca, ^{54}Ca
- Spectra, transition rates

Calcium Isotopes: Magic Numbers





GXPF1: Honma, Otsuka, Brown, Mizusaki (2004)
KB3G: Poves, Sanchez-Solano, Caurier, Nowacki (2001)



Phenomenological Forces

Large gap at ^{48}Ca

Discrepancy at *N=34*

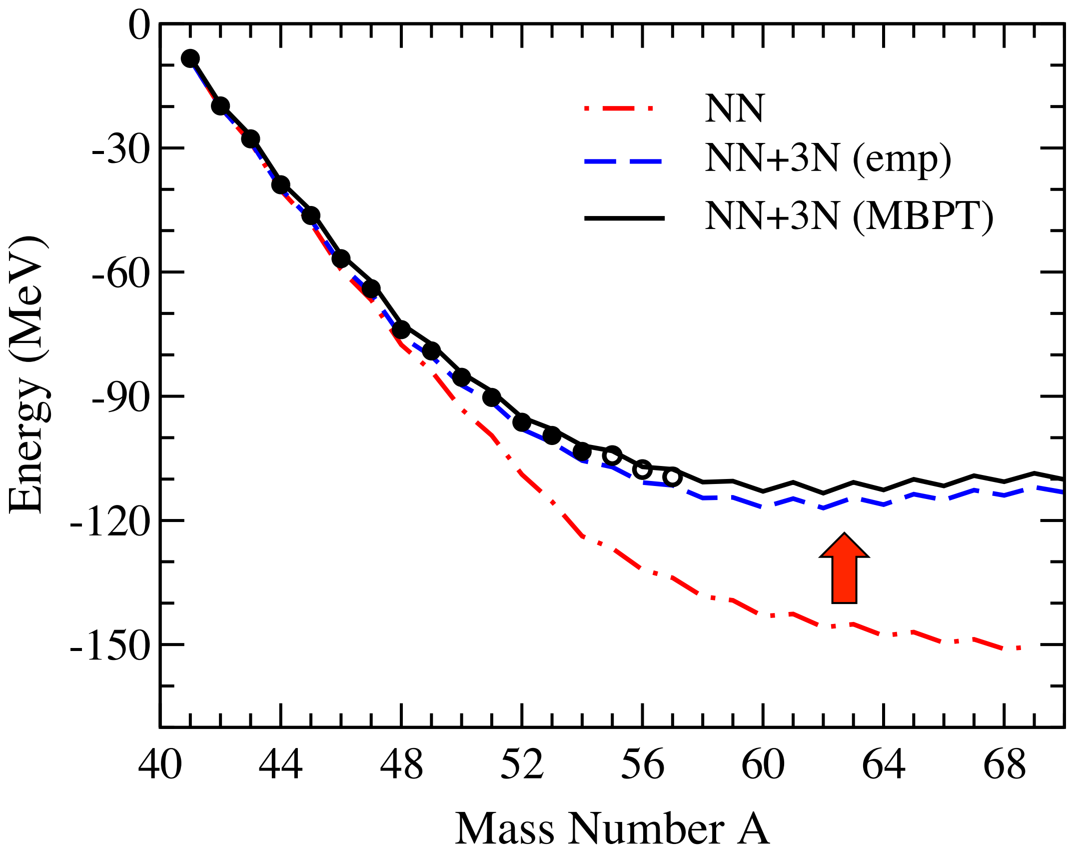
Microscopic NN Theory

Small gap at ^{48}Ca

N=28: first standard magic number not reproduced in microscopic NN theories

Calcium Ground State Energies and Dripline

Signatures of shell evolution from ground-state energies?



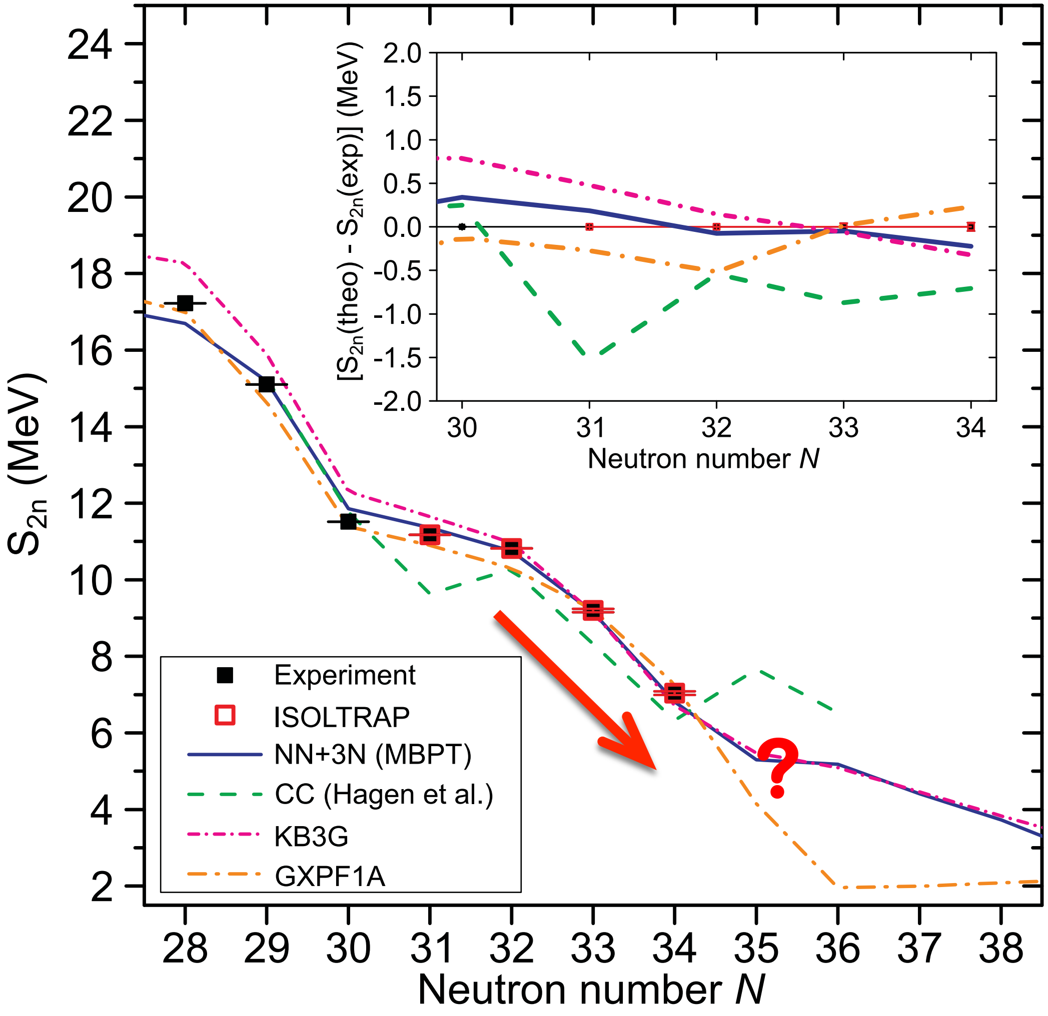
Holt, Otsuka, Schwenk, Suzuki, JPG (2012)

No clear dripline; flat behavior past ^{54}Ca – **Halos beyond ^{60}Ca?**

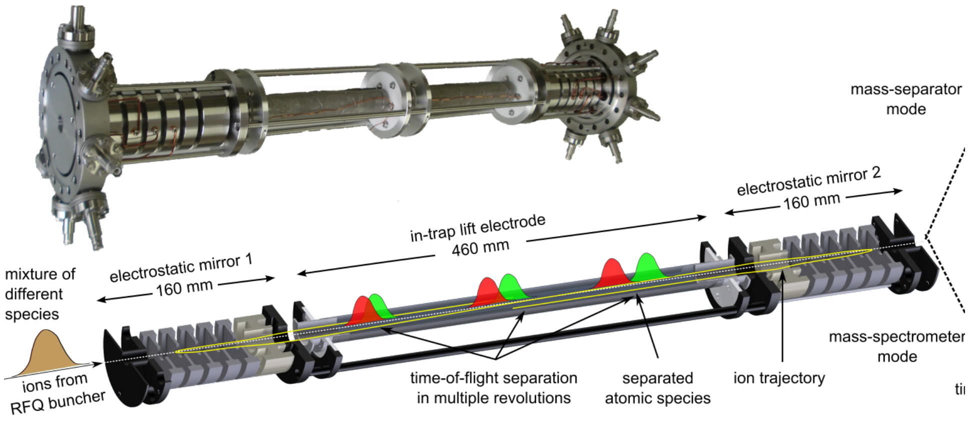
$S_{2n} = -\left[BE(N,Z) - BE(N-2,Z)\right]$ **sharp decrease indicates shell closure**

Experimental Connection: Mass of ^{54}Ca

New precision mass measurement of ^{53,54}Ca at **ISOLTRAP**: multi-reflection ToF



Wienholtz et al., Nature (2013)



ISOLTRAP ***Measurement***

Sharp decrease past ^{52}Ca

Unambiguous closed-shell ^{52}Ca

Test predictions of various models

MBPT NN+3N

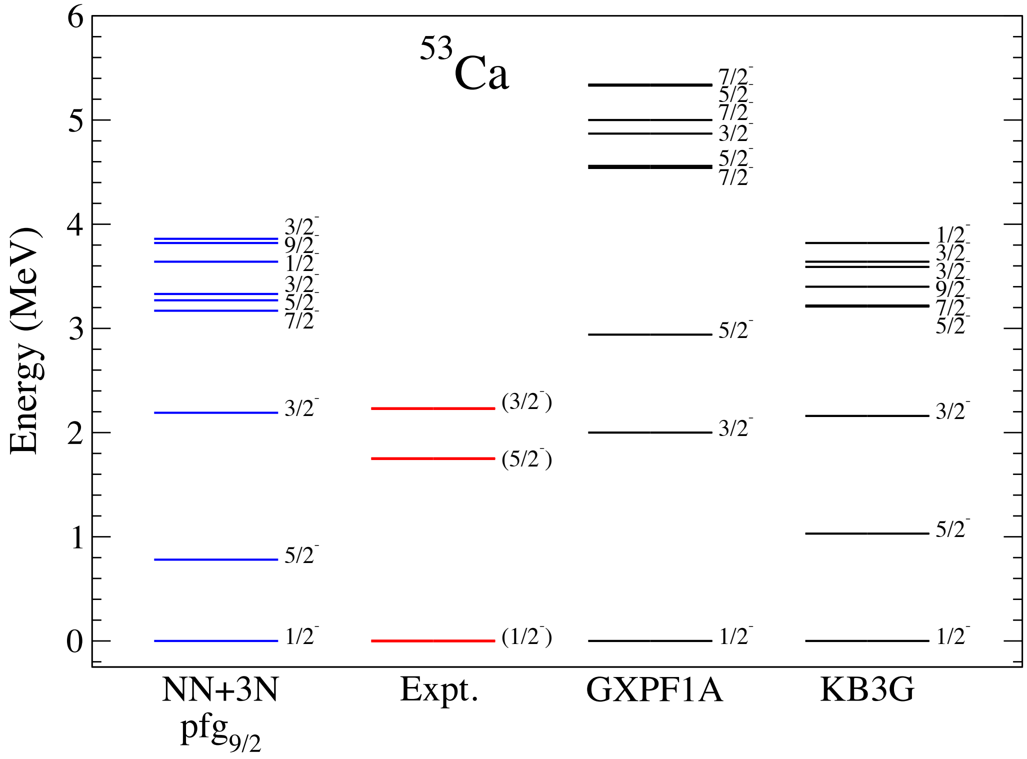
Excellent agreement with new data

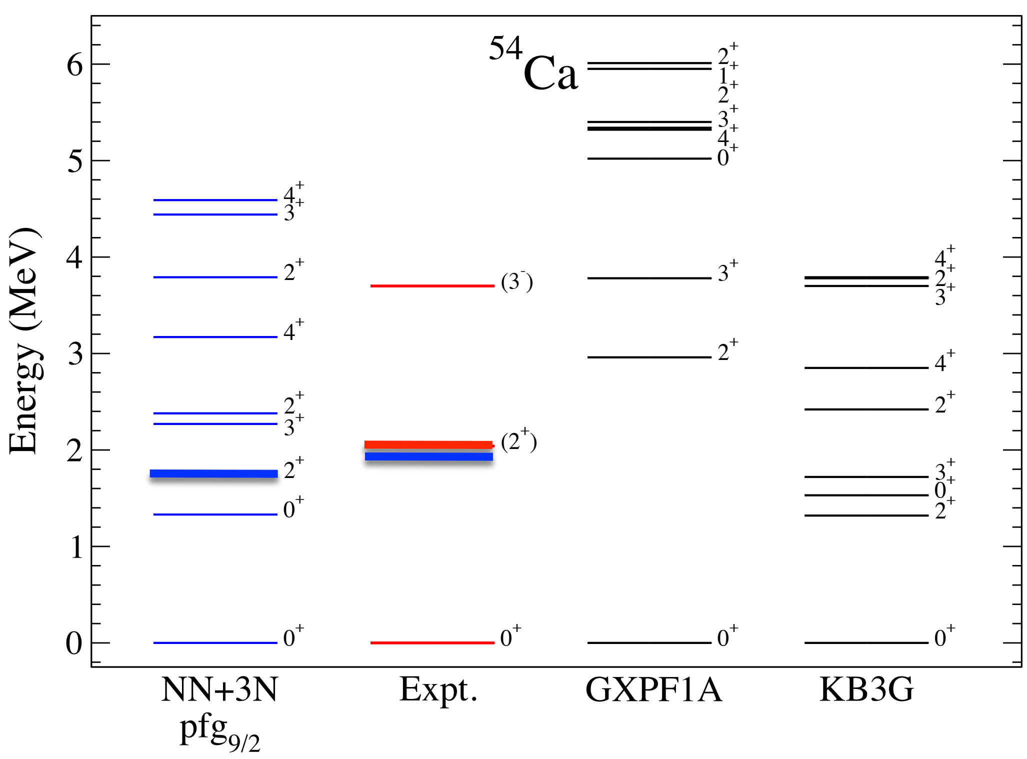
Reproduces closed-shell ^{48,52}Ca

Weak closed sell signature past ^{54}Ca

Neutron-Rich Ca Spectra Near N=34

Neutron-rich calcium spectra with NN+3N





JDH, Menendez, Schwenk, JPG (2013)
JDH, Menendez, Simonis, Schwenk, PRC (2014)
Hagen et al., PRL (2013)

Phenomenology: inconsistent predictions

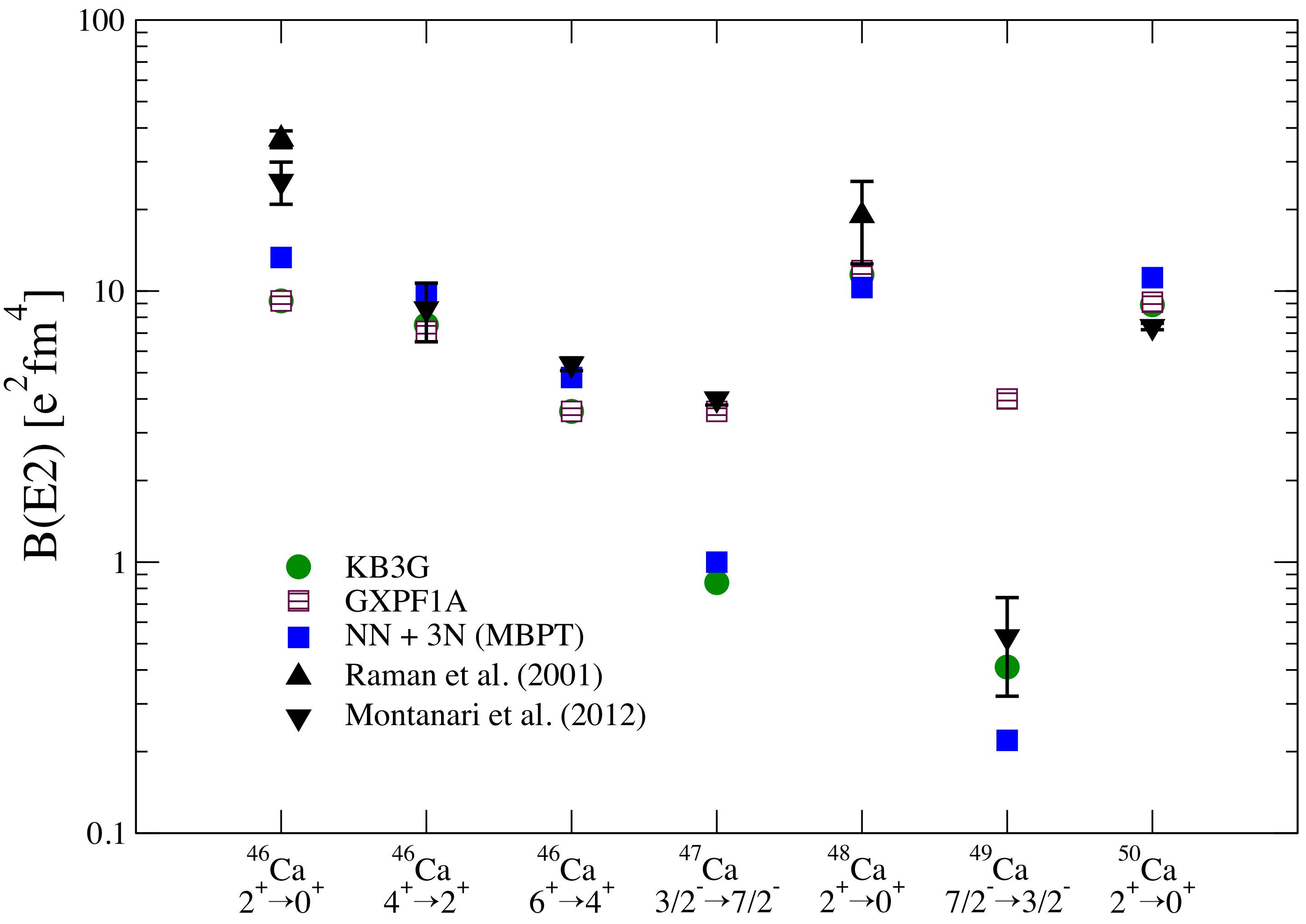
NN+3N: signature of new *N=34* magic number (also predicted in CC theory)

Agrees with new measurements from RIKEN

Steppenbeck et al., Nature (2013)

Transition Rates

Neutron-rich calcium B(E2) rates



JDH, Menendez, Simonis, Schwenk, PRC (2014)

Reasonable agreement with experiment – comparable to phenomenology

Uses effective charges – need calculated effective operators!

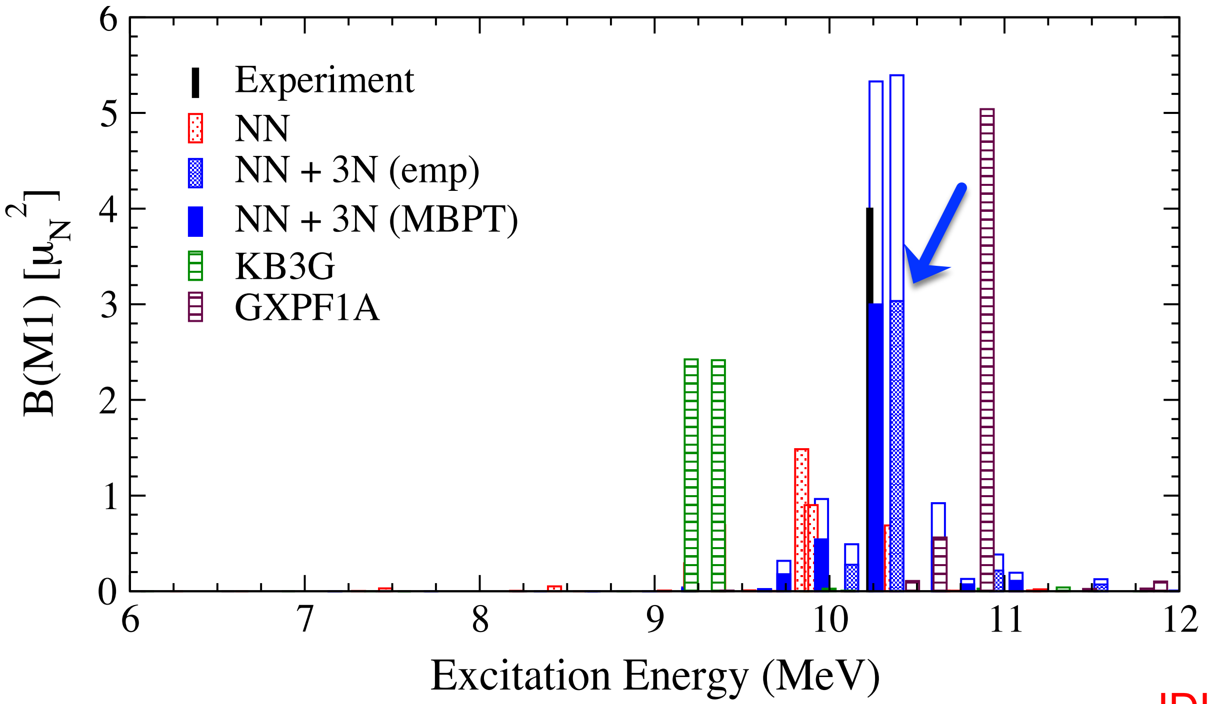
N=28 Magic Number: *M1* Transition Strength

$B(M1: 0^+_{gs} \rightarrow 1^+)$ concentration indicates a single particle (spin-flip) transition

von Neumann-Coesel, *et al*. (1998)

Not reproduced in phenomenology

NN-only: highly fragmented strength, well below experiment



JDH, Menendez, Simonis, Schwenk, PRC (2014)

$pfg_{9/2}$-shell:

3N gives additional concentration

Peak close to experimental energy

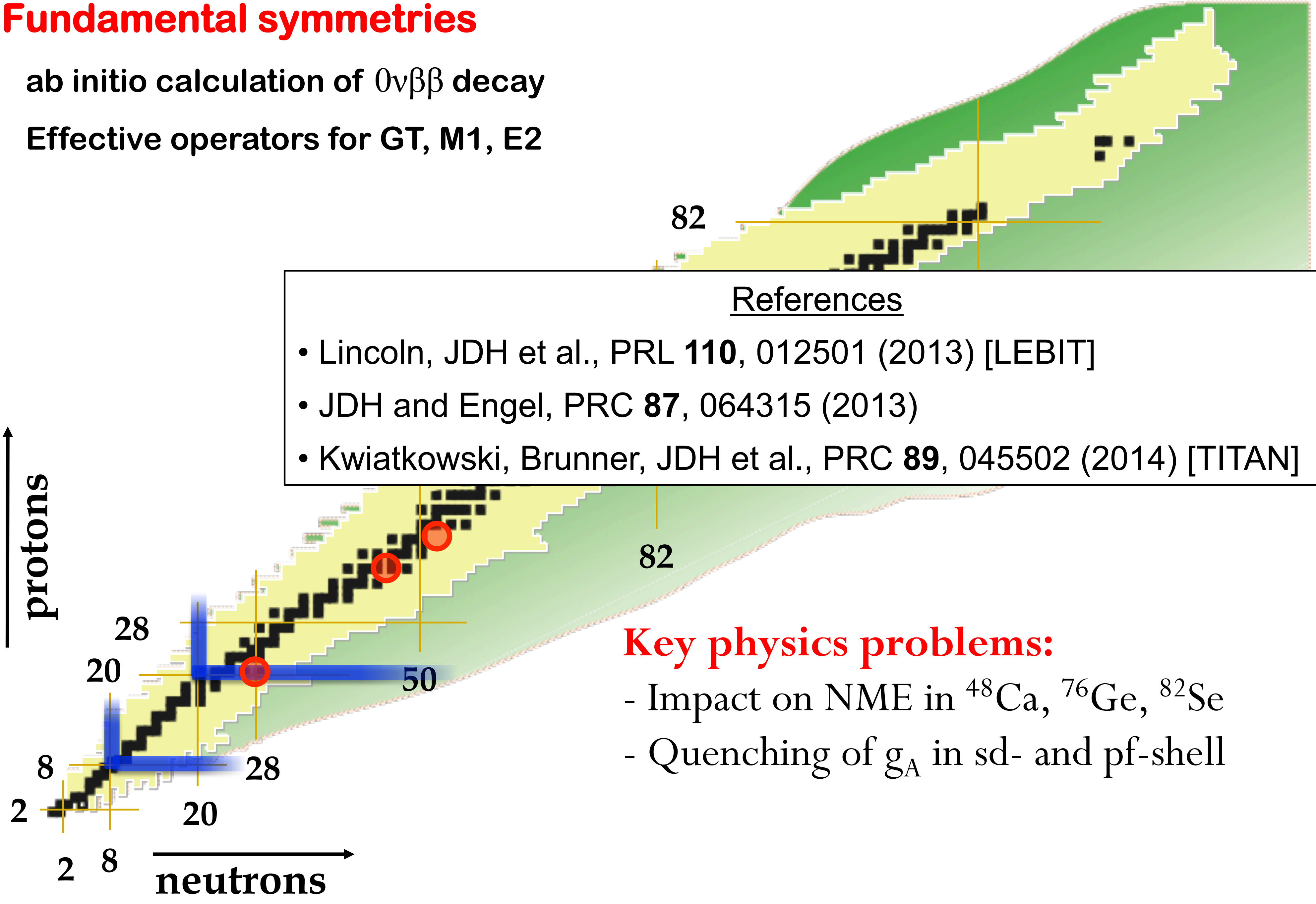
Supports *N=28* magic number

Calculations of Effective Operators

Fundamental symmetries

ab initio calculation of $0\nu\beta\beta$ decay

Effective operators for GT, M1, E2



References

- Lincoln, JDH et al., PRL **110**, 012501 (2013) [LEBIT]
- JDH and Engel, PRC **87**, 064315 (2013)
- Kwiatkowski, Brunner, JDH et al., PRC **89**, 045502 (2014) [TITAN]

Key physics problems:

- Impact on NME in ^{48}Ca, ^{76}Ge, ^{82}Se
- Quenching of g_A in sd- and pf-shell

0νββ-Decay Operator

Details of operator used in subsequent calculations

Closure approximation good to 8-10% Sen'kov, Horoi, Brown, PRC (2014)

$$M_{0\nu} = \frac{2R}{\pi g_A^2} \int_0^\infty q\, dq$$

$$\times \langle f | \sum_{a,b} \frac{j_0(q r_{ab}) [h_F(q) + h_{GT}(q) \vec{\sigma}_a \cdot \vec{\sigma}_b]}{q + \overline{E} - (E_i + E_f)/2} \tau_a^+ \tau_b^+ | i \rangle$$

$$h_F(q) \equiv -g_V^2(q^2),$$

$$h_{GT}(q) \equiv g_A^2(q^2) - \frac{g_A(q^2) g_P(q^2) q^2}{3 m_p} + \frac{g_P^2(q^2) q^4}{12 m_p^2} + \frac{g_M^2(q^2) q^2}{6 m_p^2}$$

$$g_V(q^2) = \frac{1}{[1 + q^2/(0.85\mathrm{GeV}^2)]^2} \qquad g_P(q^2) = \frac{2 m_p g_A(q^2)}{q^2 + m_\pi^2}$$

$$g_A(q^2) = \frac{1.27}{[1 + q^2/(1.09\mathrm{Gev}^2)]^2}, \qquad g_M(q^2) = 3.70 g_V(q^2)$$

1) Nuclear wavefunctions: currently phenomenological – calculate ab initio

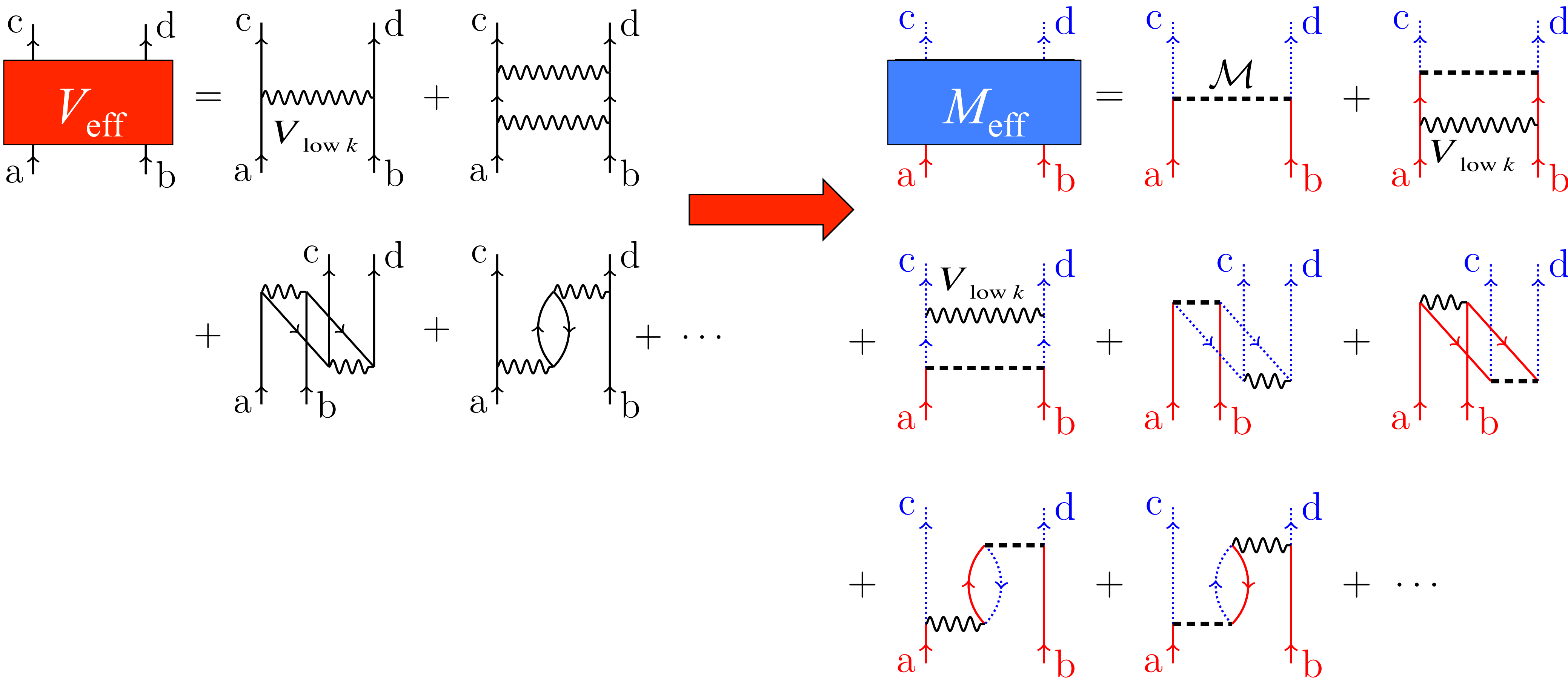
2) **Decay operator**: **correlations outside valence space**; 2-body currents

Effective 0νββ-Decay Operator

Standard approach: phenomenological wavefunctions + **bare** operator

Calculate ***effective*** 0νββ-decay operator using MBPT

Diagrammatically similar: replace one interaction vertex with $\boldsymbol{M}_{0\nu}$ operator

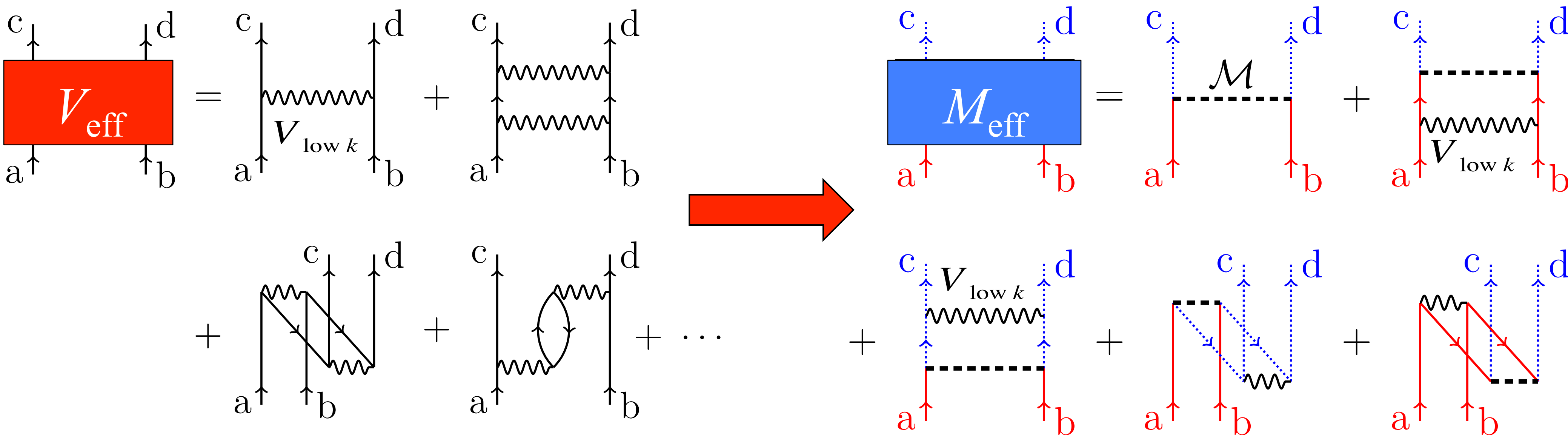


Effective 0νββ-Decay Operator

Standard approach: phenomenological wavefunctions + **bare** operator

Calculate ***effective*** 0νββ-decay operator using MBPT

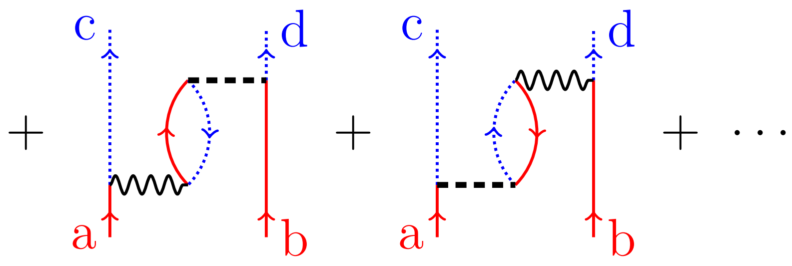
Diagrammatically similar: replace one interaction vertex with $\boldsymbol{M}_{0\nu}$ operator



Previous: G-matrix calculation to

1^{st}-order MBPT non-convergent

Engel and Hagen, PRC (2009)



Low-momentum interactions: Improve convergence behavior

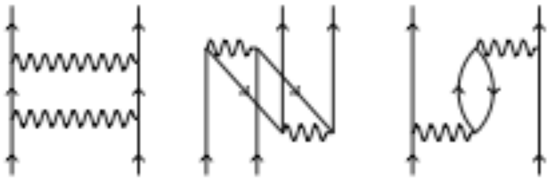
Effective 0νββ-Decay Operator

Calculate in MBPT:

1st order (× 2)

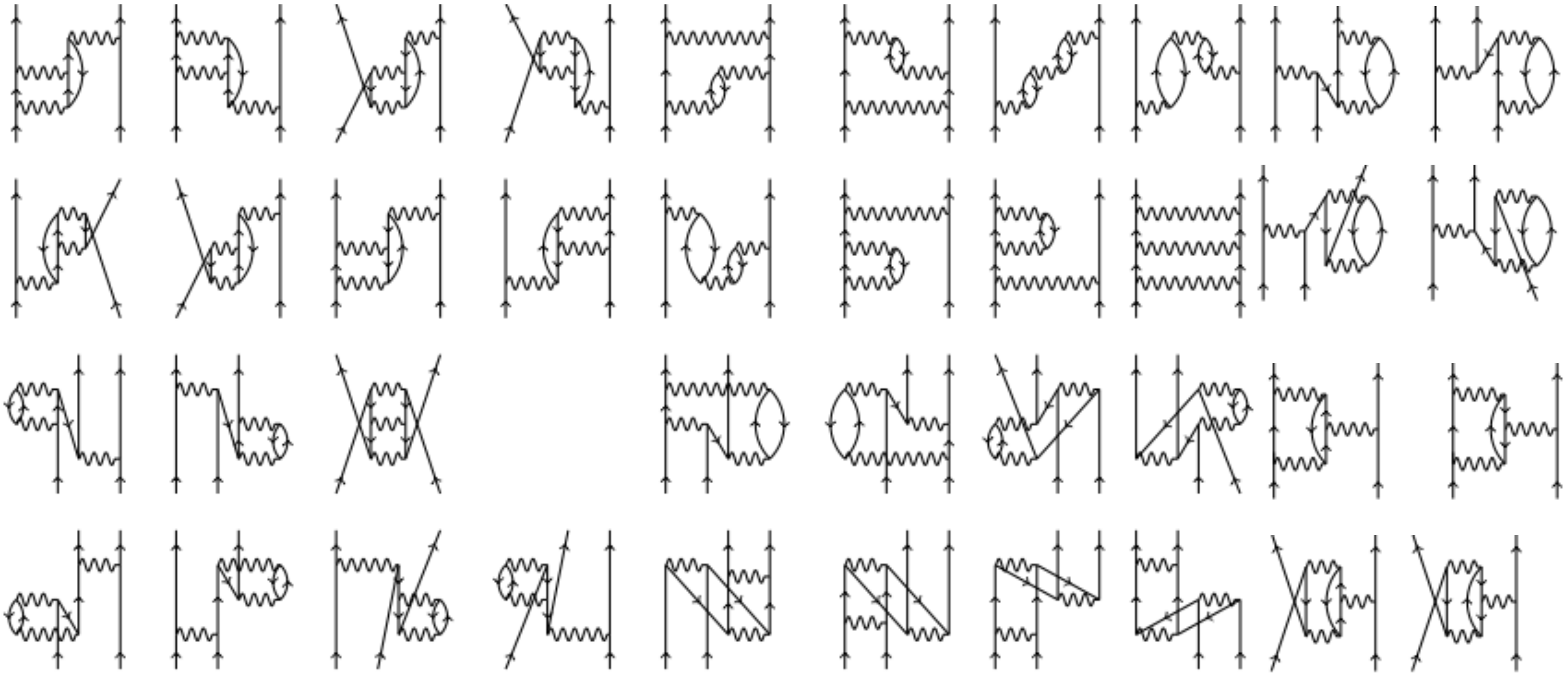
Effective 0νββ-Decay Operator

Calculate in MBPT:



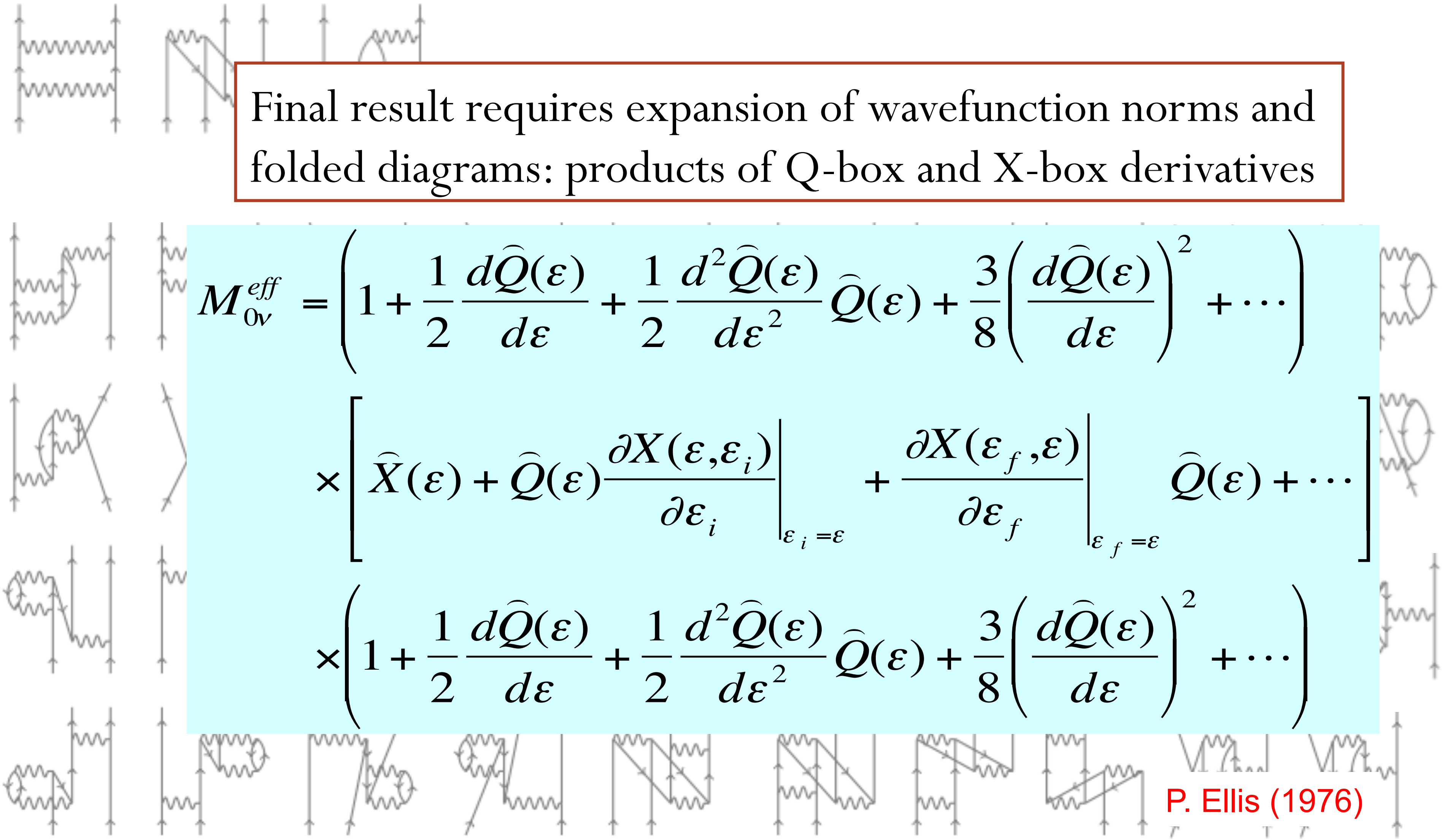
1st order (× 2)

2nd order (×3)



Effective 0νββ-Decay Operator

Calculate in MBPT:



Final result requires expansion of wavefunction norms and folded diagrams: products of Q-box and X-box derivatives

$$M_{0\nu}^{eff} = \left(1+\frac{1}{2}\frac{d\hat{Q}(\varepsilon)}{d\varepsilon}+\frac{1}{2}\frac{d^2\hat{Q}(\varepsilon)}{d\varepsilon^2}\hat{Q}(\varepsilon)+\frac{3}{8}\left(\frac{d\hat{Q}(\varepsilon)}{d\varepsilon}\right)^2+\cdots\right)$$

$$\times\left[\hat{X}(\varepsilon)+\hat{Q}(\varepsilon)\left.\frac{\partial X(\varepsilon,\varepsilon_i)}{\partial \varepsilon_i}\right|_{\varepsilon_i=\varepsilon}+\left.\frac{\partial X(\varepsilon_f,\varepsilon)}{\partial \varepsilon_f}\right|_{\varepsilon_f=\varepsilon}\hat{Q}(\varepsilon)+\cdots\right]$$

$$\times\left(1+\frac{1}{2}\frac{d\hat{Q}(\varepsilon)}{d\varepsilon}+\frac{1}{2}\frac{d^2\hat{Q}(\varepsilon)}{d\varepsilon^2}\hat{Q}(\varepsilon)+\frac{3}{8}\left(\frac{d\hat{Q}(\varepsilon)}{d\varepsilon}\right)^2+\cdots\right)$$

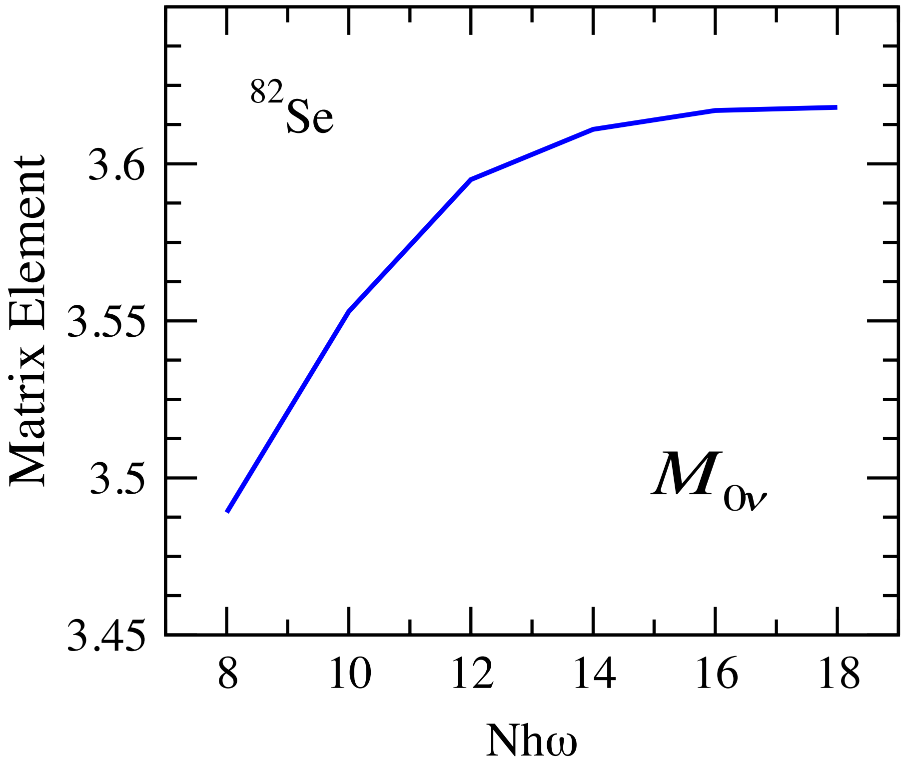
P. Ellis (1976)

Q-box – sum of interaction diagrams

X-box – sum of 0νββ diagrams

Intermediate-State Convergence

Convergence results in ^{82}Se



JDH and Engel, PRC (2013)

Results **well converged** in terms of intermediate state excitations

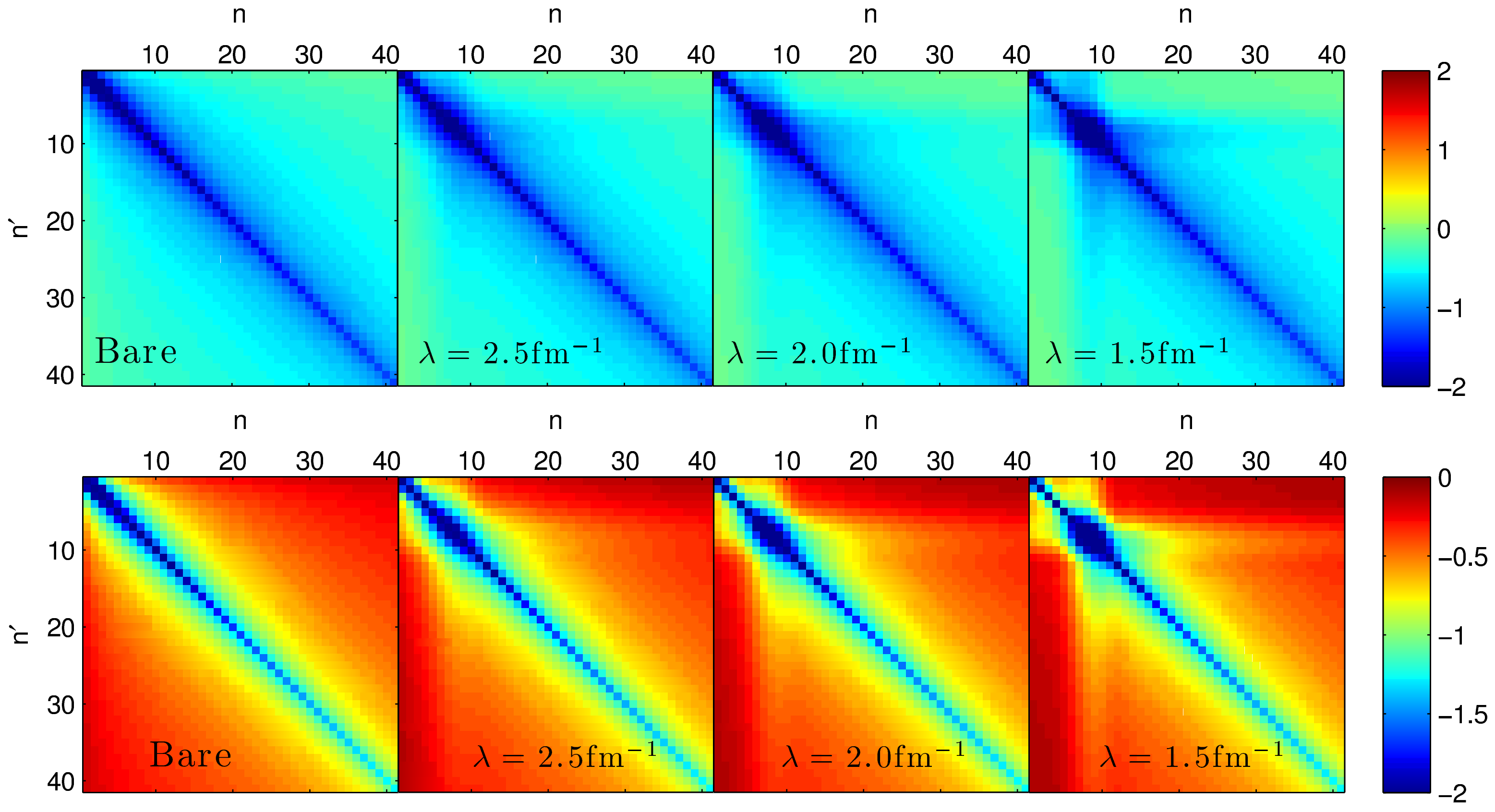
Improvement due to low-momentum interactions

Similar trend in ^{76}Ge and ^{48}Ca

Improvements from SRG-evolved operator?

SRG Evolution of Operator

Promising preliminary results with schematic of 0νββ operator



Schuster et al

Full 0νββ operator in progress

Forthcoming: test in effective-operator calculations

Calculations of $M_{0\nu}$ in ^{82}Se and ^{76}Ge

Phenomenological wavefunctions from A. Poves, M. Horoi ($pf_{5/2}\,g_{9/2}$ space)

^{76}Ge	Bare matrix element	**3.12**
	Full 1st order	**3.11**
	Full 2nd order	**3.77**

^{82}Se	Bare matrix element	**2.73**
	Full 1st order	**2.79**
	Full 2nd order	**3.62**

Converged in 13 major oscillator shells

Little net effect at 1st order

Lincoln, JDH et al., PRL (2013) [LEBIT]

JDH and Engel, PRC (2013)

Overall ~25-30% increase from bare value

Calculations of $M_{0\nu}$ in ^{48}Ca

Phenomenological wavefunctions from GXPF1A (standard *pf*-shell)

^{48}Ca	GT	Fermi	Tensor	**Sum**
Bare	0.675	0.130	−0.072	**0.733**
Final	1.211	0.160	−0.070	**1.301**

Kwiatkowski, Brunner, JDH et al., PRC (2014)

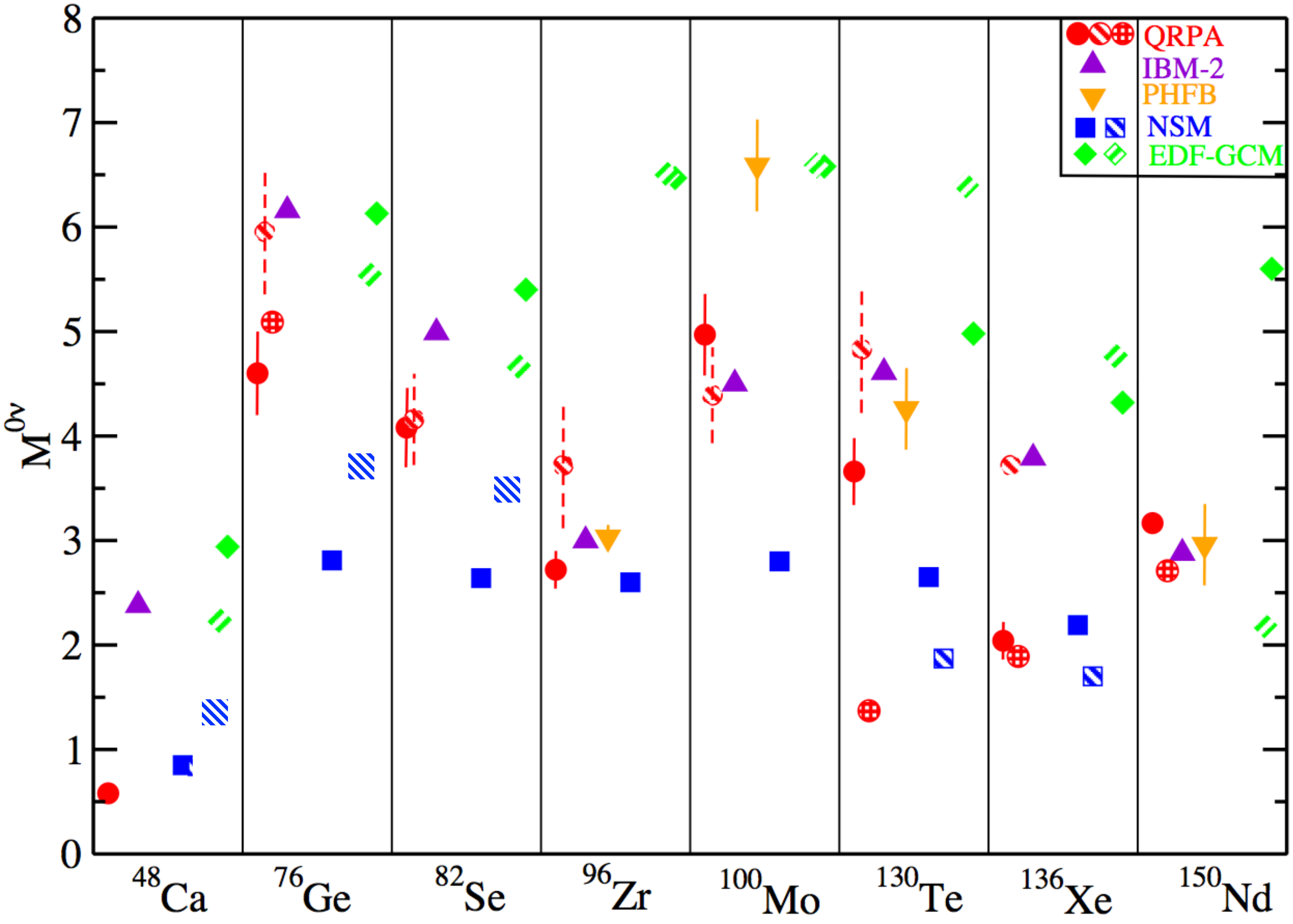
Converged in 13 major oscillator shells

Little net effect at 1st order – larger effect from 2nd order than in Ge, Se

Overall ~75% increase from bare value

Nuclear Matrix Element

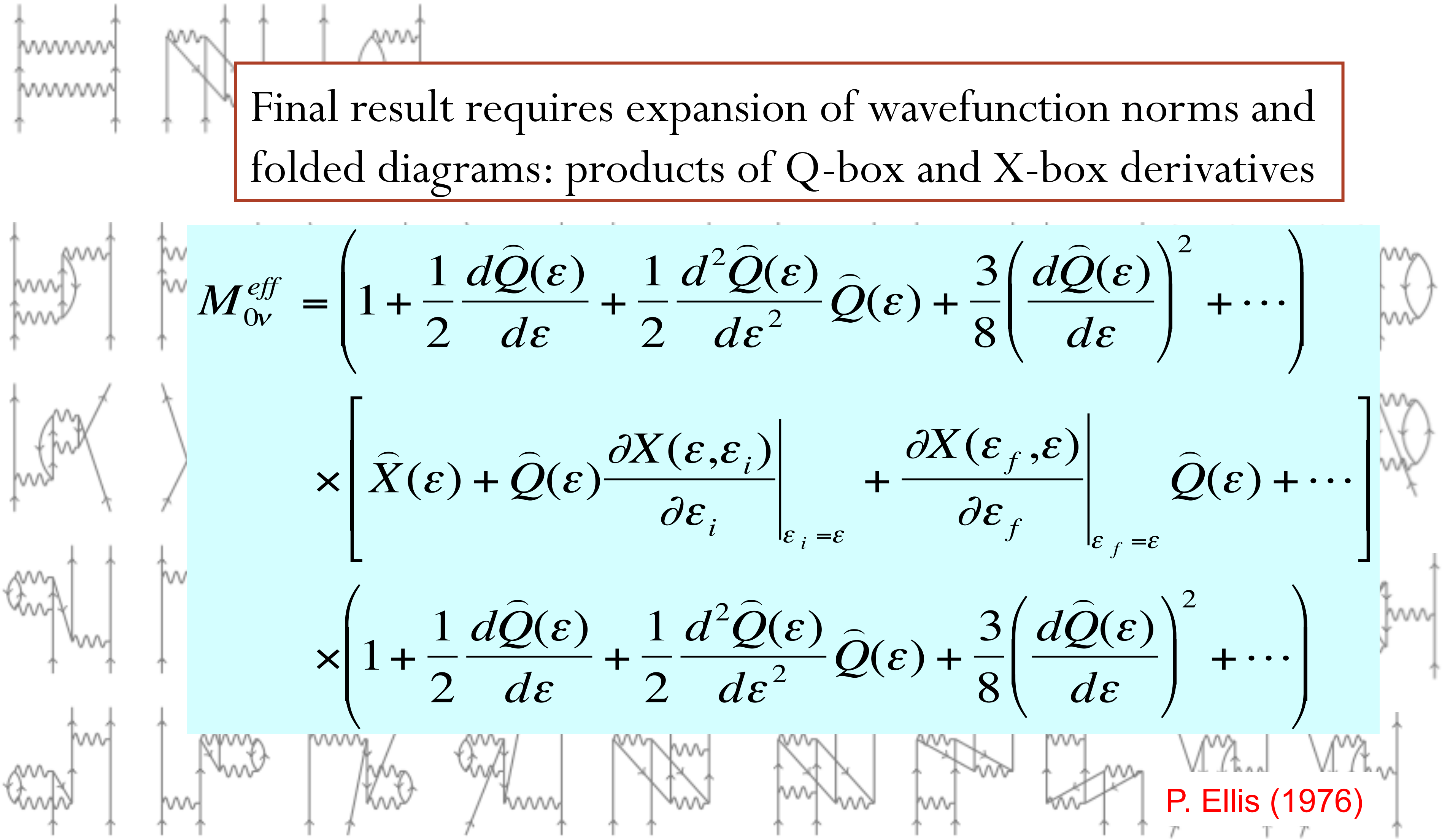
Improved calculations move in direction of other methods



Aim: first-principles framework capable of robust prediction

Effective 0νββ-Decay Operator

Calculate in MBPT:



Final result requires expansion of wavefunction norms and folded diagrams: products of Q-box and X-box derivatives

$$
\begin{aligned}
M_{0\nu}^{eff} = & \left(1 + \frac{1}{2}\frac{d\hat{Q}(\varepsilon)}{d\varepsilon} + \frac{1}{2}\frac{d^2\hat{Q}(\varepsilon)}{d\varepsilon^2}\hat{Q}(\varepsilon) + \frac{3}{8}\left(\frac{d\hat{Q}(\varepsilon)}{d\varepsilon}\right)^2 + \cdots\right) \\
& \times\left[\hat{X}(\varepsilon) + \hat{Q}(\varepsilon)\frac{\partial X(\varepsilon,\varepsilon_i)}{\partial \varepsilon_i}\bigg|_{\varepsilon_i=\varepsilon} + \frac{\partial X(\varepsilon_f,\varepsilon)}{\partial \varepsilon_f}\bigg|_{\varepsilon_f=\varepsilon}\hat{Q}(\varepsilon) + \cdots\right] \\
& \times\left(1 + \frac{1}{2}\frac{d\hat{Q}(\varepsilon)}{d\varepsilon} + \frac{1}{2}\frac{d^2\hat{Q}(\varepsilon)}{d\varepsilon^2}\hat{Q}(\varepsilon) + \frac{3}{8}\left(\frac{d\hat{Q}(\varepsilon)}{d\varepsilon}\right)^2 + \cdots\right)
\end{aligned}
$$

P. Ellis (1976)

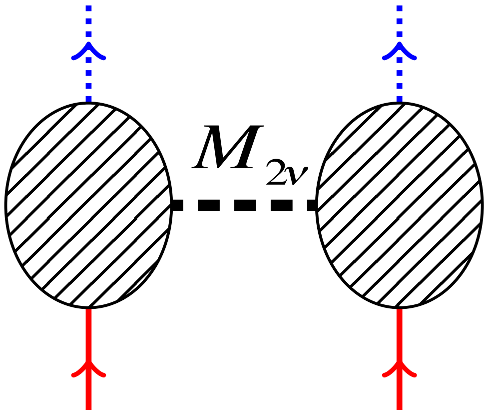
Q-box – sum of interaction diagrams

X-box – sum of 0νββ diagrams

Quenching of GT Strength

Investigate many-body effects on quenching of g_A

Set of two-body diagrams contributing to renormalization of g_A in $2\nu\beta\beta$ decay: product of 2 single-beta-decay

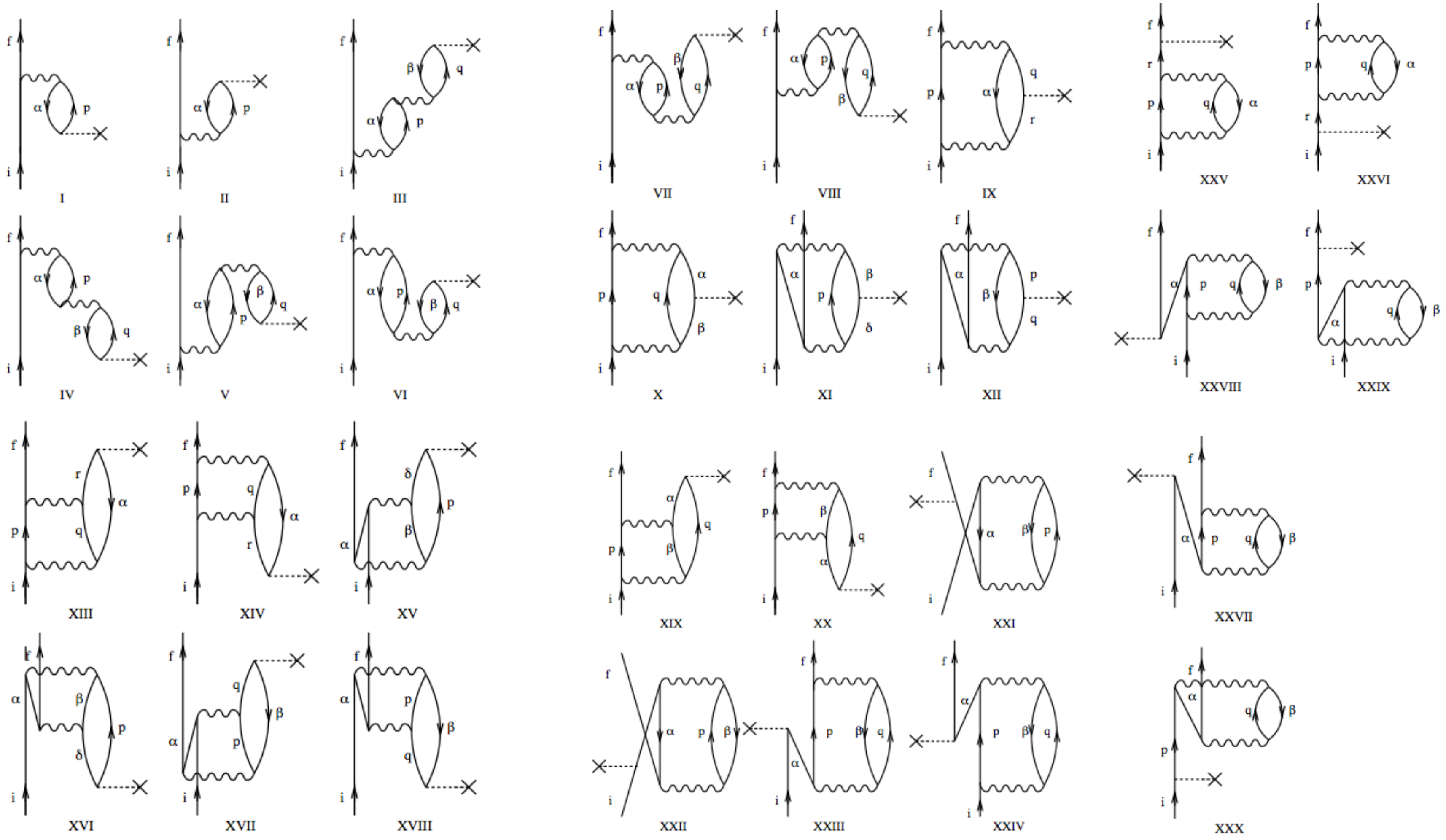


Quenching of 38% in ^{82}Se ($g_A \sim 1.0$)

Quenching of GT Strength

Investigate many-body effects on quenching of g_A

Directly look at one-body effective GT

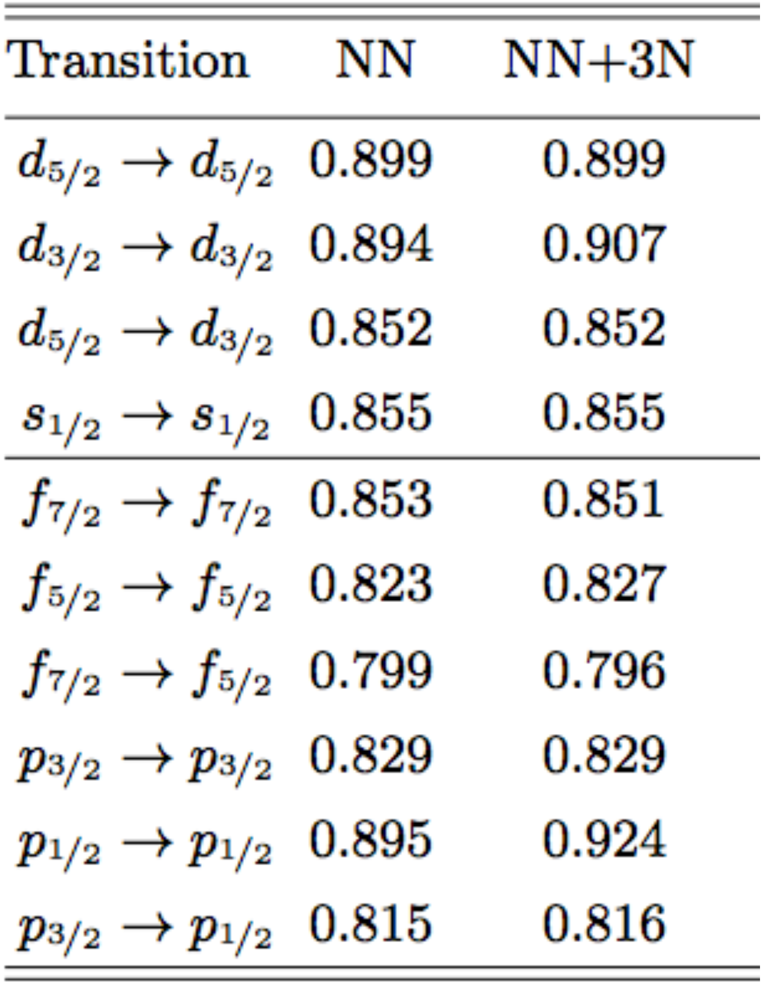


Use low-momentum interactions and 3N forces

Quenching of GT Strength

Investigate many-body effects on quenching of g_A

Calculate GT transitions in sd- and pf-shells



Transition	NN	NN+3N
$d_{5/2} \rightarrow d_{5/2}$	0.899	0.899
$d_{3/2} \rightarrow d_{3/2}$	0.894	0.907
$d_{5/2} \rightarrow d_{3/2}$	0.852	0.852
$s_{1/2} \rightarrow s_{1/2}$	0.855	0.855
$f_{7/2} \rightarrow f_{7/2}$	0.853	0.851
$f_{5/2} \rightarrow f_{5/2}$	0.823	0.827
$f_{7/2} \rightarrow f_{5/2}$	0.799	0.796
$p_{3/2} \rightarrow p_{3/2}$	0.829	0.829
$p_{1/2} \rightarrow p_{1/2}$	0.895	0.924
$p_{3/2} \rightarrow p_{1/2}$	0.815	0.816

Net quenching between 0.8-0.9

Consistent with findings from $2\nu\beta\beta$ decay

Larger quenching when spin-orbit partners absent from valence space

Converged using low-momentum interactions – little effect from 3N

Conclusion/Outlook

- Nuclear structure theory of medium-mass nuclei with 3N forces, extended spaces
- Robust repulsive 3N mechanism for T=1 neutron/proton-rich nuclei
- **Calcium isotopes** in *pf*- and $pfg_{9/2}$-shells:
  - Prediction of $N=28$ magic number in ^{48}Ca
  - Shell evolution towards the dripline: small $N=34$ closure
  - Pairing gaps reflect shell structure – higher-order many-body processes essential
  - NN+3N predictions confirmed in new TITAN and ISOLTRAP experiments

- New directions for fundamental symmetries
  - Effective operators for 0vBB decay
  - 30% increase for Ge, Se; 75% increase for ^{48}Ca
  - Effective one-body GT: quenching 0.8-0.9
  - Many improvements needed

Path to Full Calculation

Benchmark in 48Ca

Ab initio valence-shell Hamiltonians

Towards full sd- and pf-shells

Revisit cross-shell theory

Moving beyond stability

Continuum effects near driplines

Islands of inversion in sd/pf regions

Exotic cores

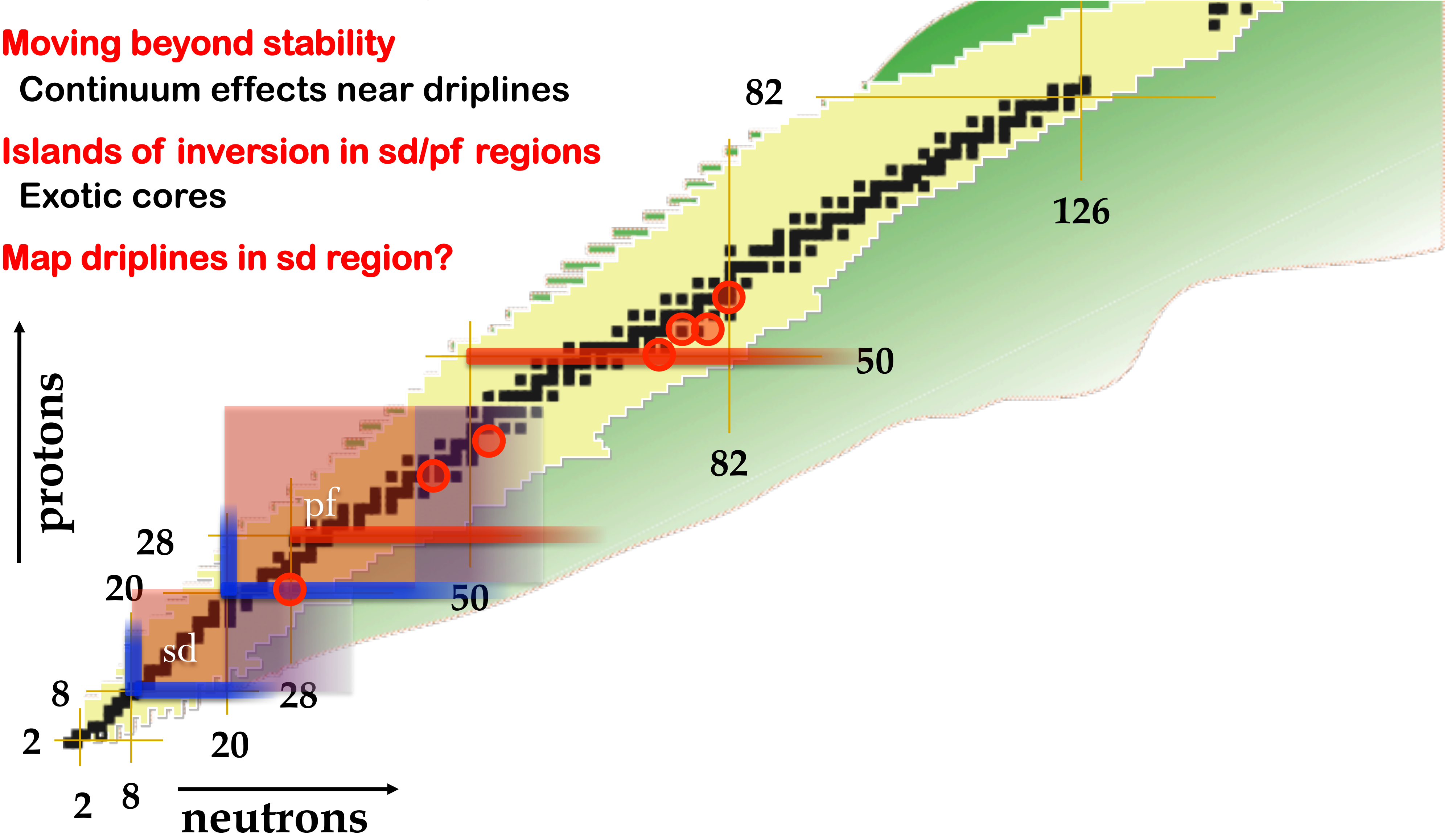
Map driplines in sd region?

Fundamental symmetries

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

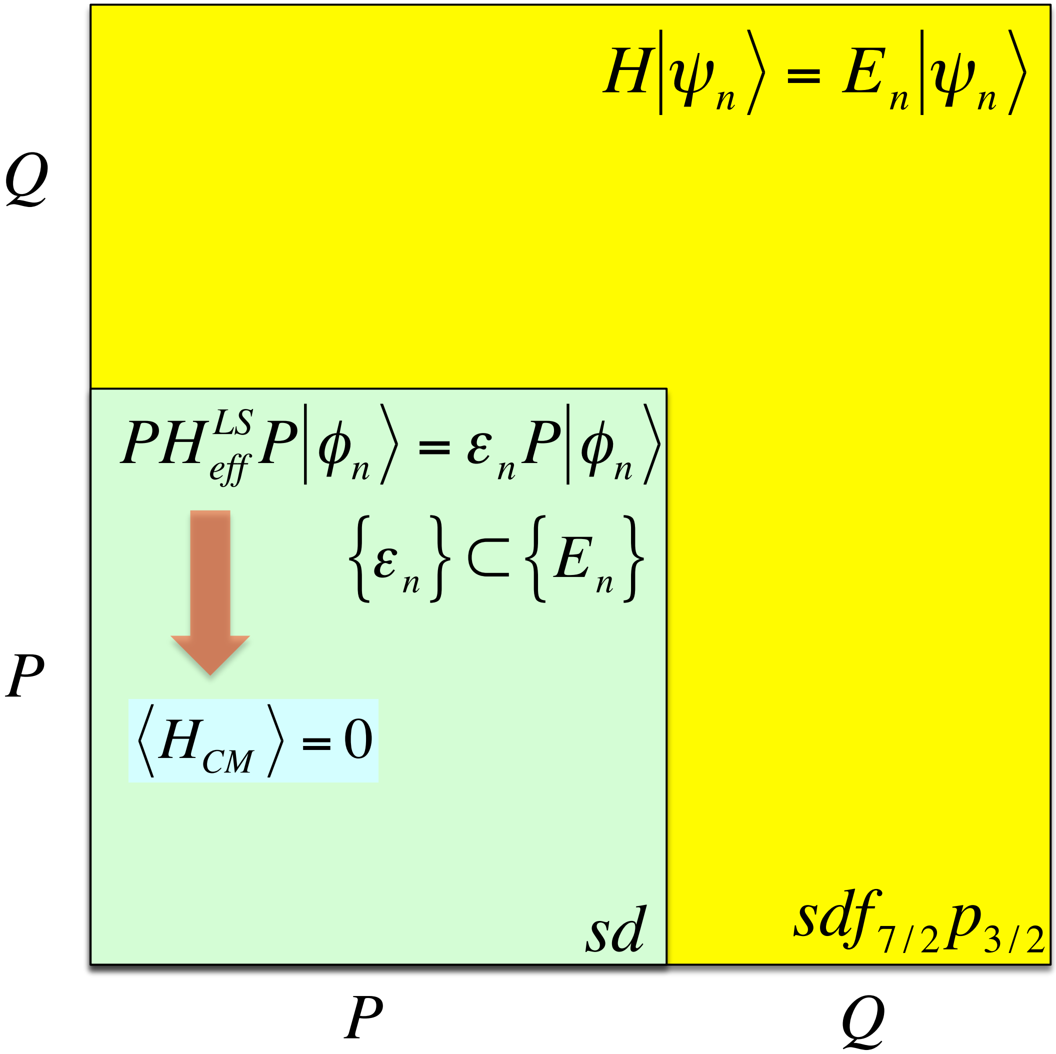
Effective electroweak operators

WIMP-nucleus scattering



Evaluating Center-of-Mass Contamination

Nonperturbative Lee-Suzuki (LS) transformation from extended space



$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

$$PH_{eff}^{LS}P|\phi_n\rangle = \varepsilon_n P|\phi_n\rangle$$

$$\{\varepsilon_n\} \subset \{E_n\}$$

$$\langle H_{CM}\rangle = 0$$

Transform for **two-body** systems ($e.g.$, ^{18}O, ^{42}Ca)

Extended-space spectrum free of CM contamination

Project into standard space onto eigenenergies from extended space calculation

Use H_{eff}^{LS} as new two-body Hamiltonian in *sd*-shell valence-space calculations

Calculations of $M_{0\nu}$ in ^{82}Se and ^{76}Ge

Calculation of ^{82}Se (phenomenological wavefunctions from A. Poves, M. Horoi)

^{76}Ge	Bare matrix element	3.12
+	pp, hh ladders (1st)	5.44
+	3p-1h	2.20
+	2nd-order	4.14

^{82}Se	Bare matrix element	2.73
+	pp, hh ladders (1st)	4.86
+	3p-1h	2.40
+	2nd-order	3.92

JDH and Engel, PRC (2013)

Large effects cancel at 1st order

Conclusion/Outlook

- Nuclear structure theory of medium-mass nuclei with 3N forces, extended spaces

- **Non-empirical valence-space methods**
  - First calculations based on NN+3N forces
  - Extended valence spaces needed
  - Cures NN-only failings: dripline, shell evolution, spectra
  - Residual 3N forces improve predictions beyond dripline

- **New directions**
  - Promising first results for F/Ne ground states to
  - Non-perturbative IM-SRG – excellent binding energies, spectra in sd shell only!

- **Large-space ab-initio methods**
  - Similar improvements with NN+3N as in valence-space methods
  - Agreement between methods encouraging for future – benchmarking valuable!

Nuclear Matrix Element

$$M_{0\nu} = M_{0\nu}^{GT} - \frac{g_V^2}{g_A^2} M_{0\nu}^{F} + \cdots$$

$$M_{0\nu}^{GT} = \langle f | \sum_{ab} H(r_{ab}) \vec{\sigma}_a \cdot \vec{\sigma}_b \tau_a^+ \tau_b^+ | i \rangle \quad M_{0\nu}^{F} = \langle f | \sum_{ab} H(r_{ab}) \tau_a^+ \tau_b^+ | i \rangle$$

Shell model: arbitrary correlations in truncated single-particle space

QRPA: simple correlations in large single-particle space

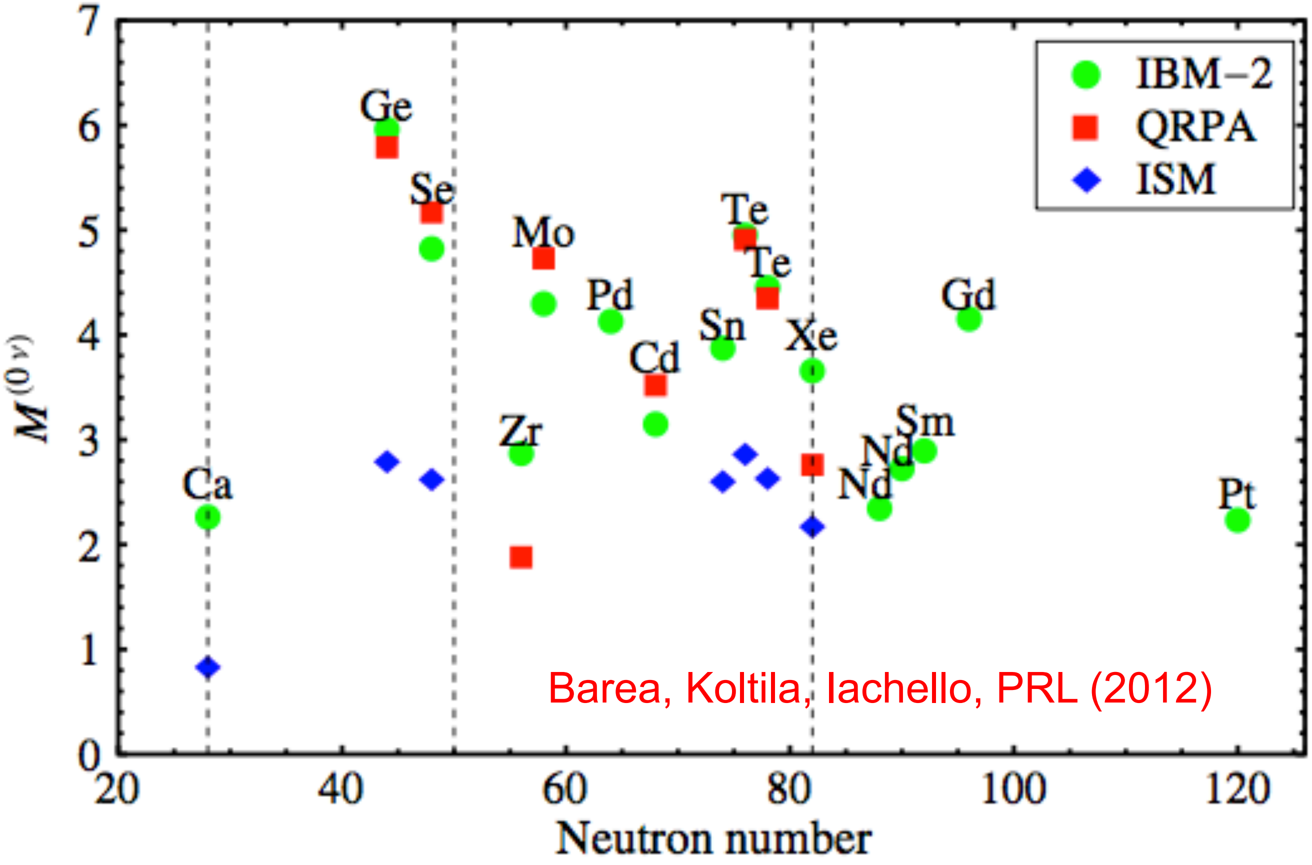
Nuclear Matrix Element

$$M_{0\nu} = M_{0\nu}^{GT} - \frac{g_V^2}{g_A^2} M_{0\nu}^{F} + \cdots$$

$$M_{0\nu}^{GT} = \langle f | \sum_{ab} H(r_{ab}) \vec{\sigma}_a \cdot \vec{\sigma}_b \tau_a^+ \tau_b^+ | i \rangle \quad M_{0\nu}^{F} = \langle f | \sum_{ab} H(r_{ab}) \tau_a^+ \tau_b^+ | i \rangle$$

Shell model: arbitrary correlations in truncated single-particle space

QRPA: simple correlations in large single-particle space



Barea, Koltila, Iachello, PRL (2012)

Pronounced differences for lighter candidates

Explore shell model improvements

Backup Oxygen

Drip Lines and Magic Numbers: 3N Forces in Medium-Mass Nuclei

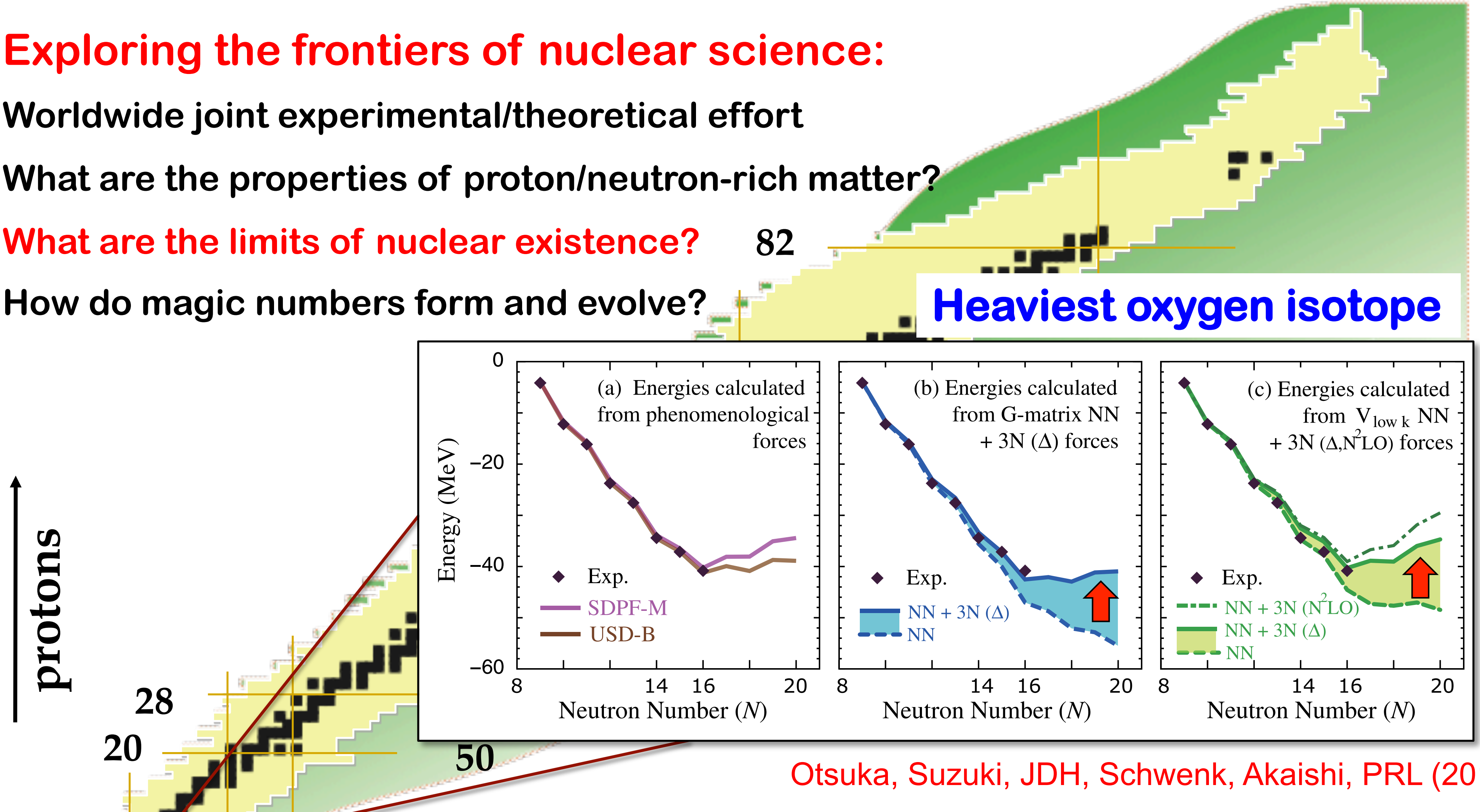
Exploring the frontiers of nuclear science:

Worldwide joint experimental/theoretical effort

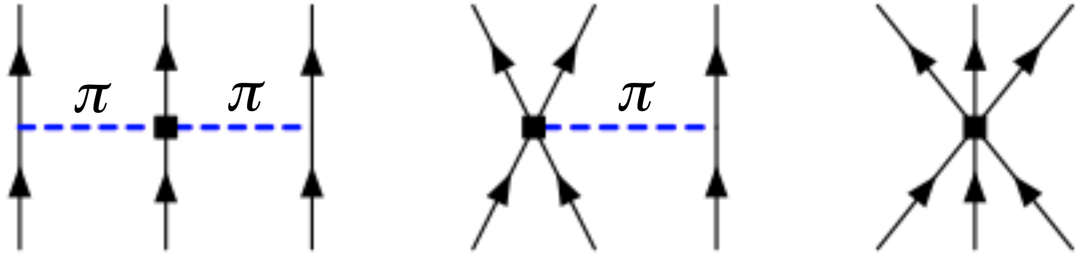
What are the properties of proton/neutron-rich matter?

What are the limits of nuclear existence?

How do magic numbers form and evolve?



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



Drip Lines and Magic Numbers:
3N Forces in Medium-Mass Nuclei

Exploring the frontiers of nuclear science:

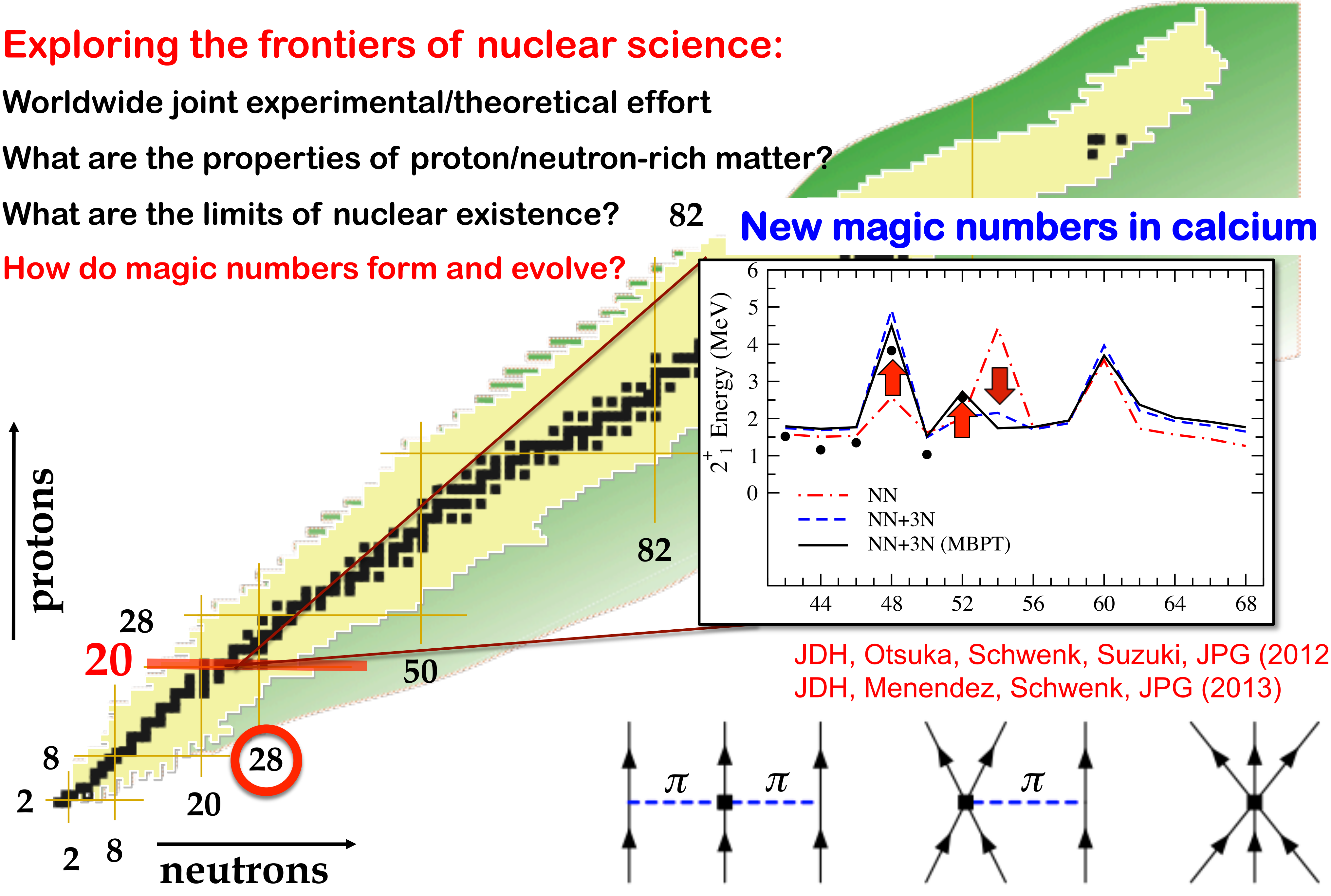
Worldwide joint experimental/theoretical effort

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

What are the limits of nuclear existence?

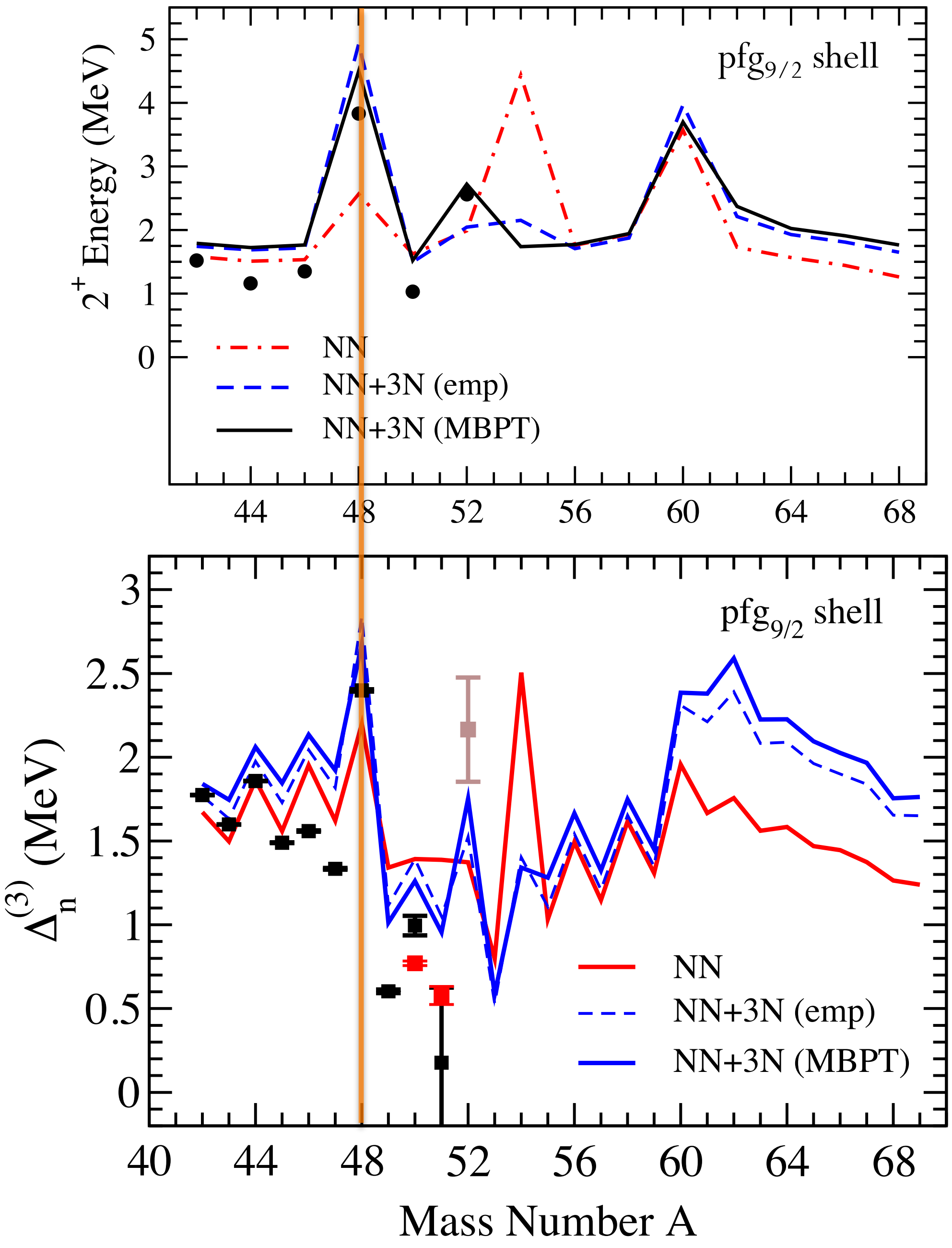
How do magic numbers form and evolve?

New magic numbers in calcium



JDH, Otsuka, Schwenk, Suzuki, JPG (2012)
JDH, Menendez, Schwenk, JPG (2013)

Pairing for Shell Evolution N=28



Peak in pairing gaps: complementary signature for shell closure

Compare with 2^+ energies for Ca

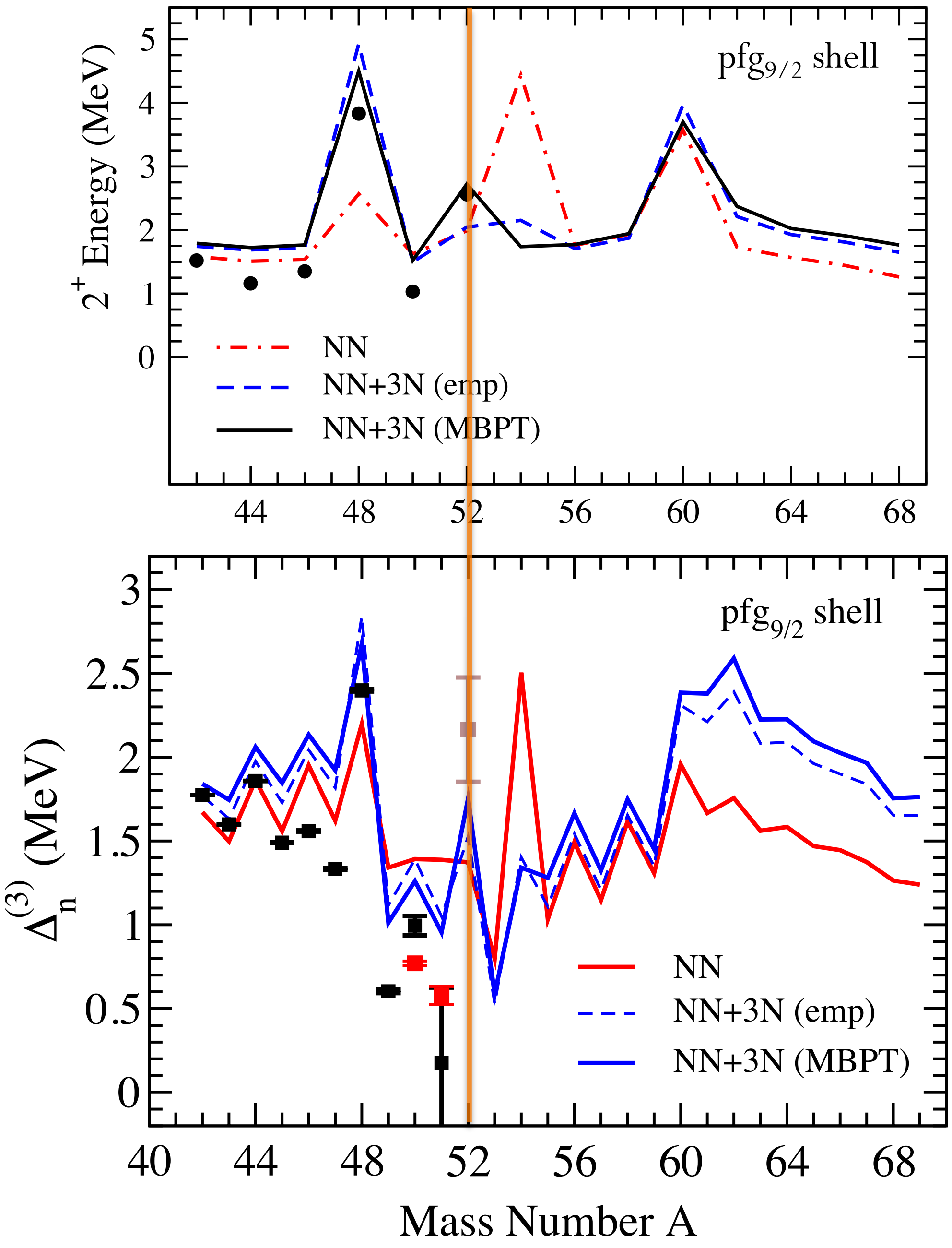
Agreement with CC throughout chain

Hagen et al. PRL (2012)

N=28 strong peak

JDH, Menendez, Schwenk, JPG (2013)

Pairing for Shell Evolution N=32



Peak in pairing gaps: complementary signature for shell closure

Compare with 2^+ energies for Ca

Agreement with CC throughout chain

Hagen et al. PRL (2012)

N=28 strong peak

N=32 moderate peak

Close to data with new TITAN value

Experimental measurement of ^{53}Ca mass needed to reduce uncertainty

JDH, Menendez, Schwenk, JPG (2013)

Oxygen Isotopes

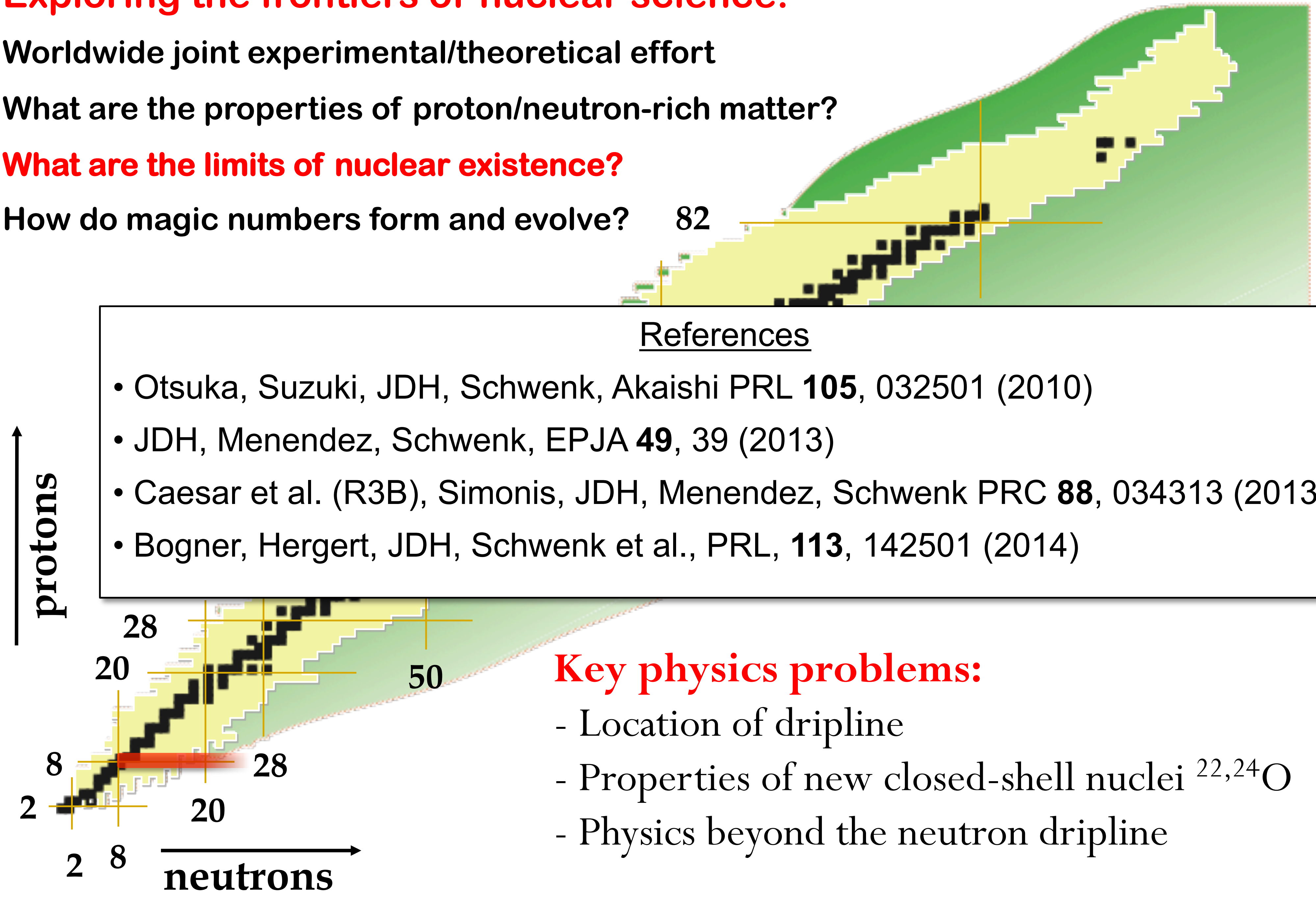
Exploring the frontiers of nuclear science:

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?



References

- Otsuka, Suzuki, JDH, Schwenk, Akaishi PRL **105**, 032501 (2010)
- JDH, Menendez, Schwenk, EPJA **49**, 39 (2013)
- Caesar et al. (R3B), Simonis, JDH, Menendez, Schwenk PRC **88**, 034313 (2013)
- Bogner, Hergert, JDH, Schwenk et al., PRL, **113**, 142501 (2014)

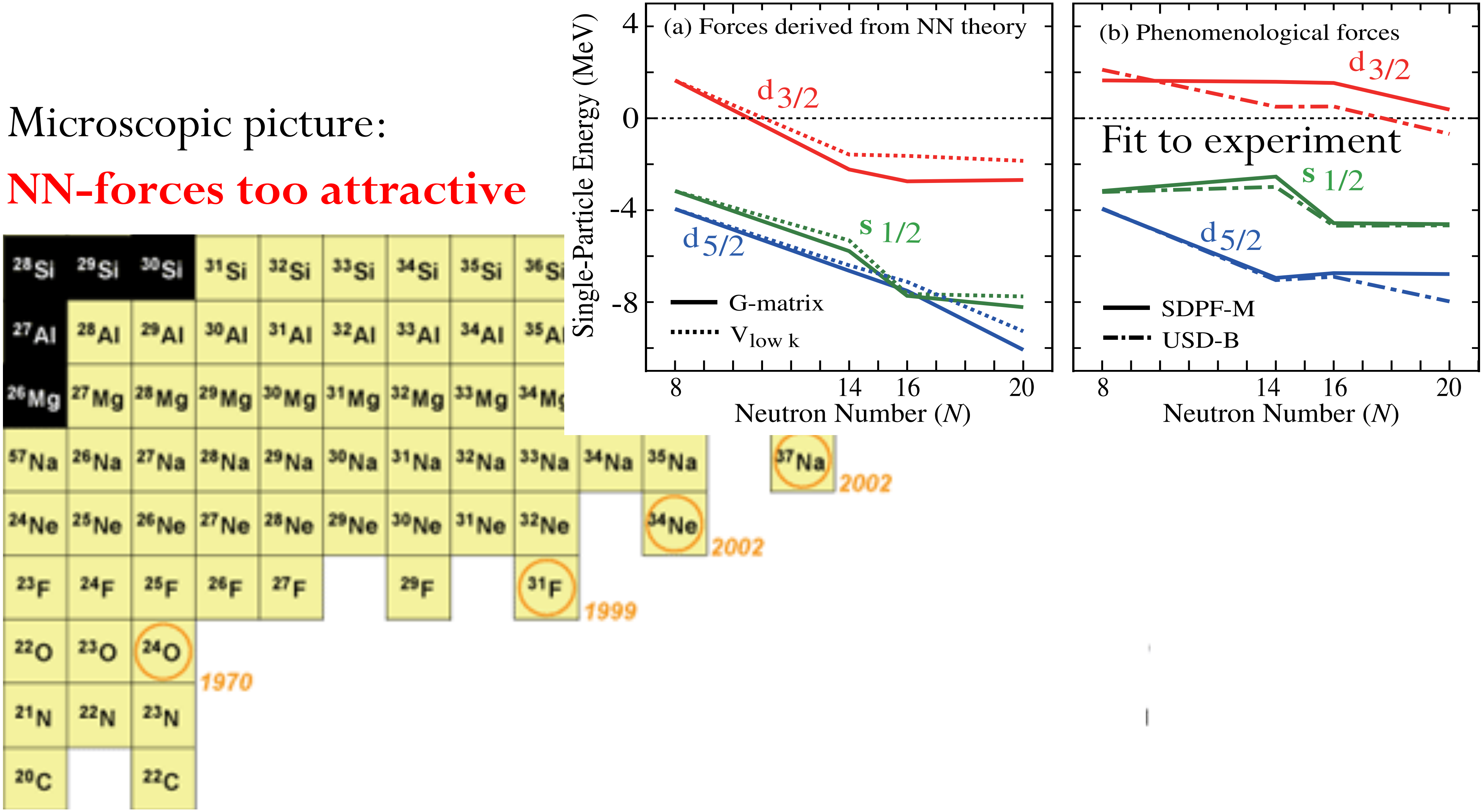
Key physics problems:

- Location of dripline
- Properties of new closed-shell nuclei ^{22,24}O
- Physics beyond the neutron dripline

Limits of Nuclear Existence: Oxygen Anomaly

Microscopic picture:

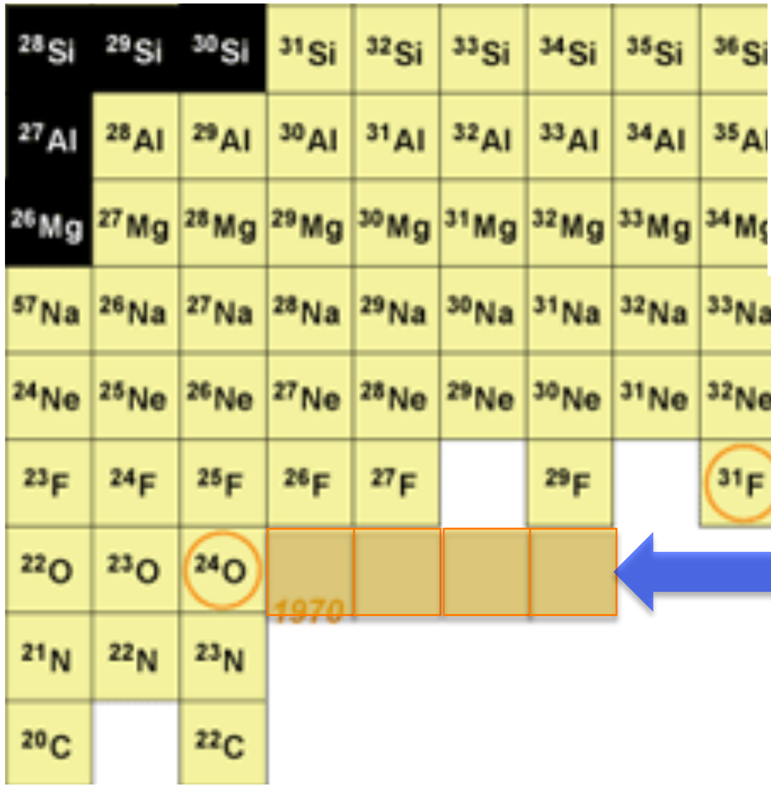
NN-forces too attractive



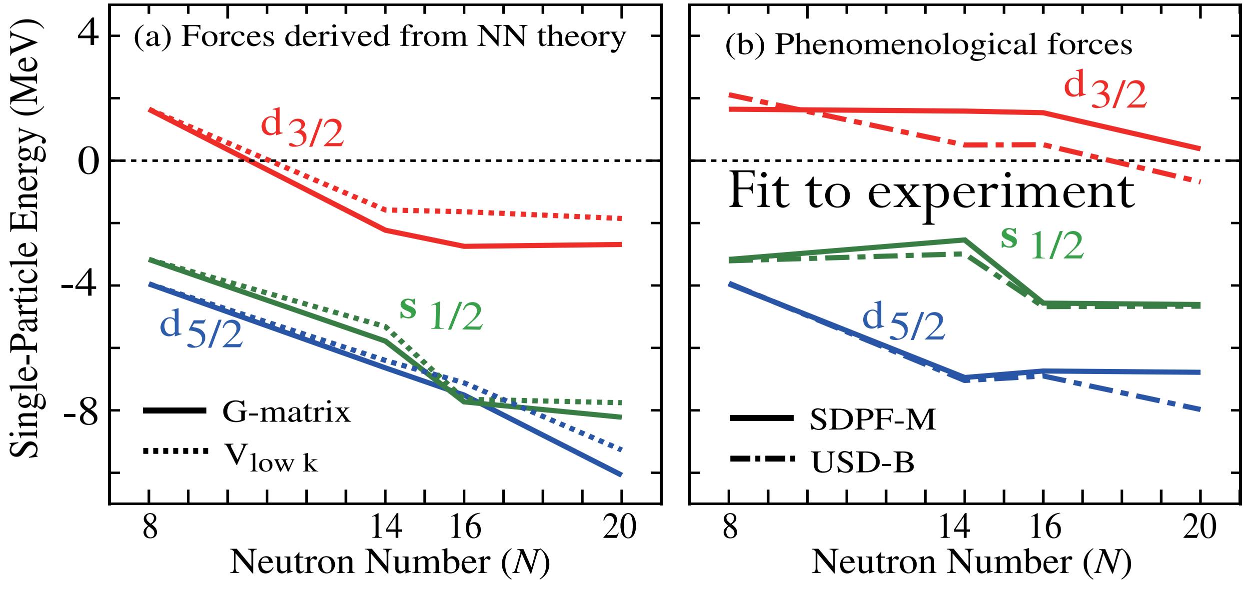
Limits of Nuclear Existence: Oxygen Anomaly

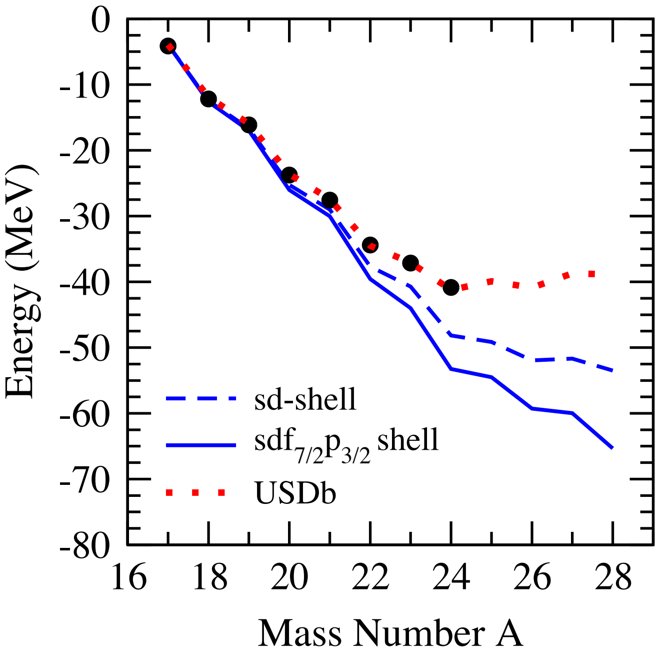
Microscopic picture:

NN-forces too attractive



NN prediction



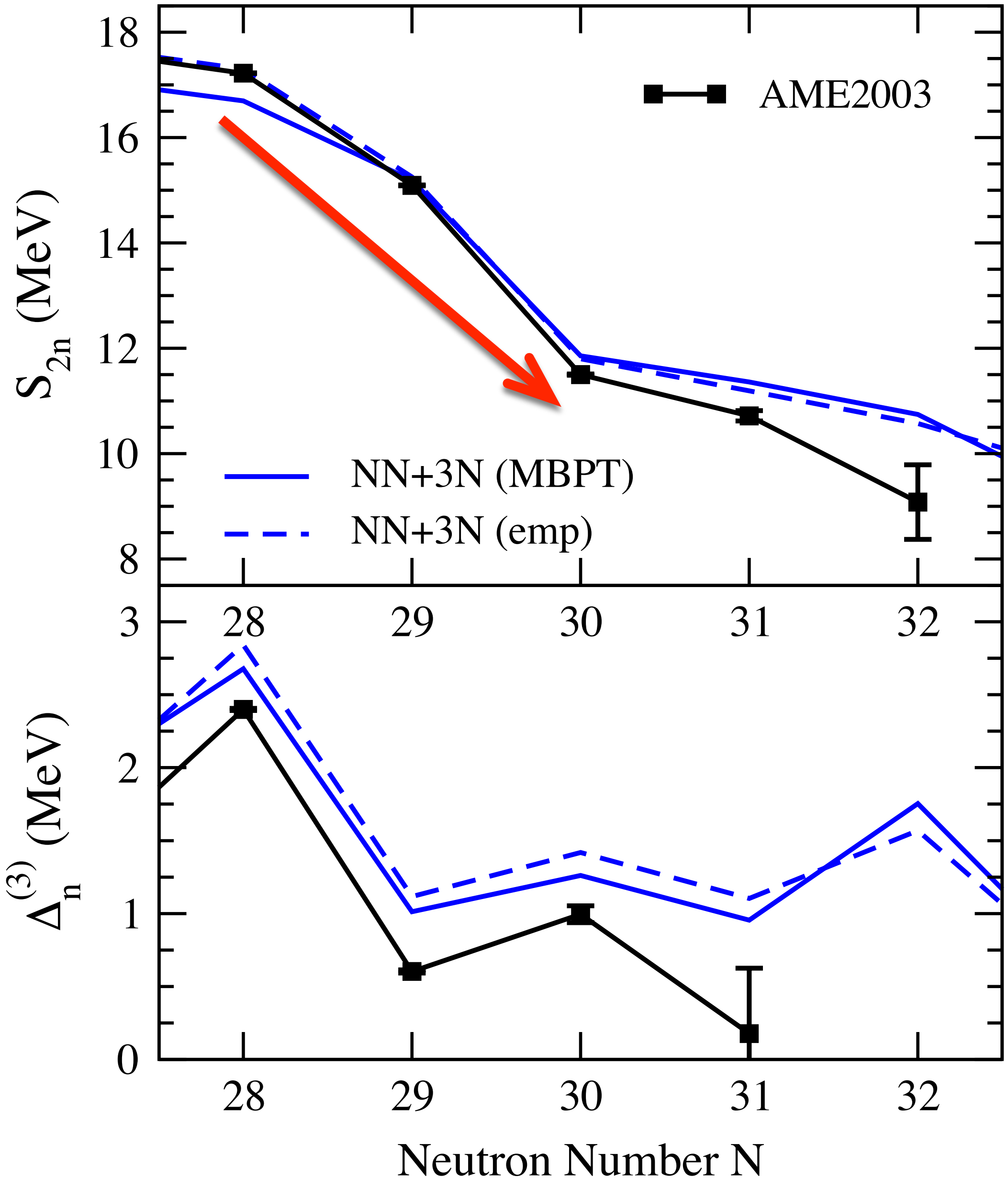


Incorrect prediction of oxygen dripline

Extended-space – more binding

Two-Neutron Separation Energies: Mass of ^{52}Ca

Compare with AME2003 data



NN+3N Predictions

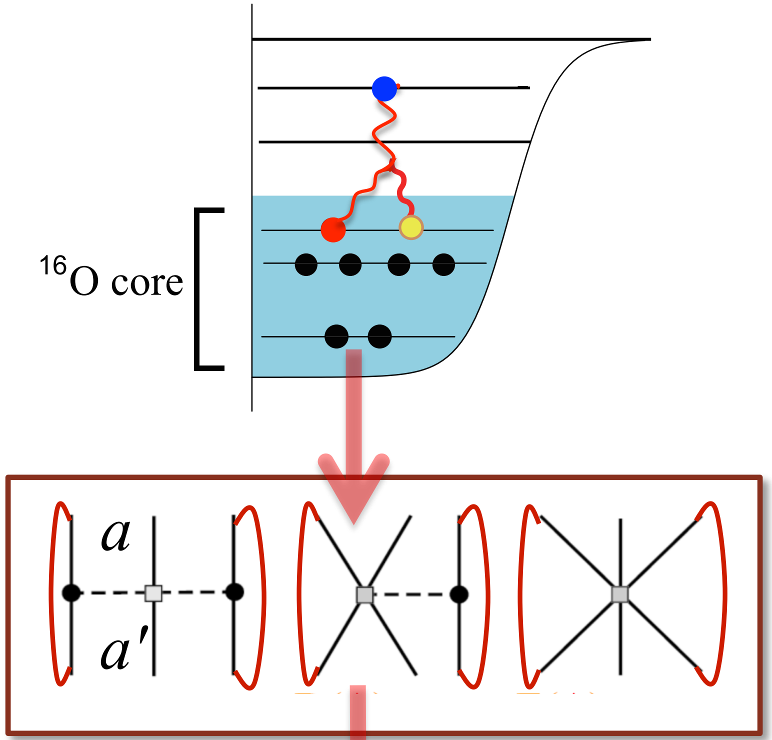
Reproduce ^{48}Ca shell closure

Predictions too bound past ^{50}Ca

3N Forces for Valence-Shell Theories

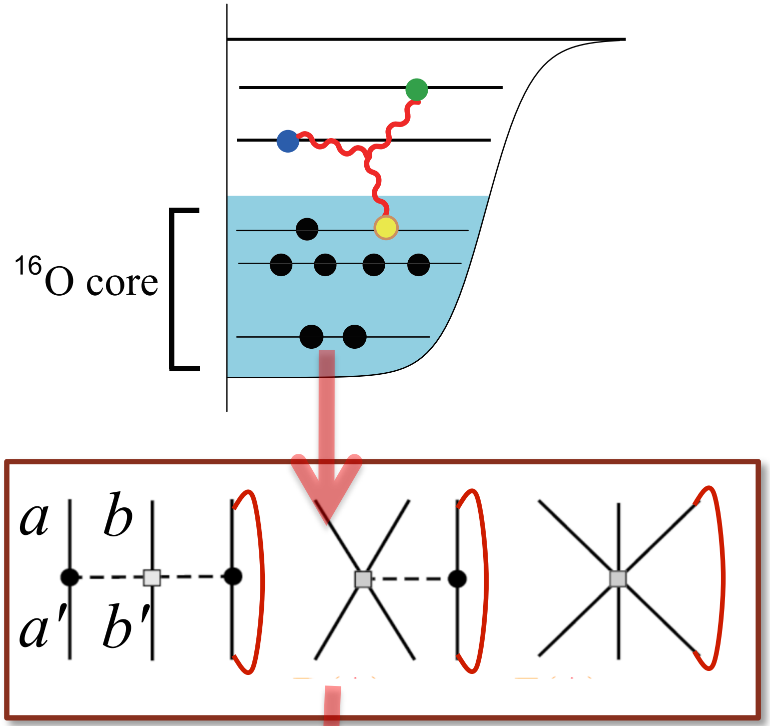
Normal-ordered 3N: contribution to valence-space Hamiltonian

Effective one-body



$$\langle a | \, V_{3N,\mathrm{eff}} \, | a' \rangle = \frac{1}{2} \sum_{\alpha\beta = core} \langle \alpha\beta a | \, V_{3N} \, | \alpha\beta a' \rangle$$

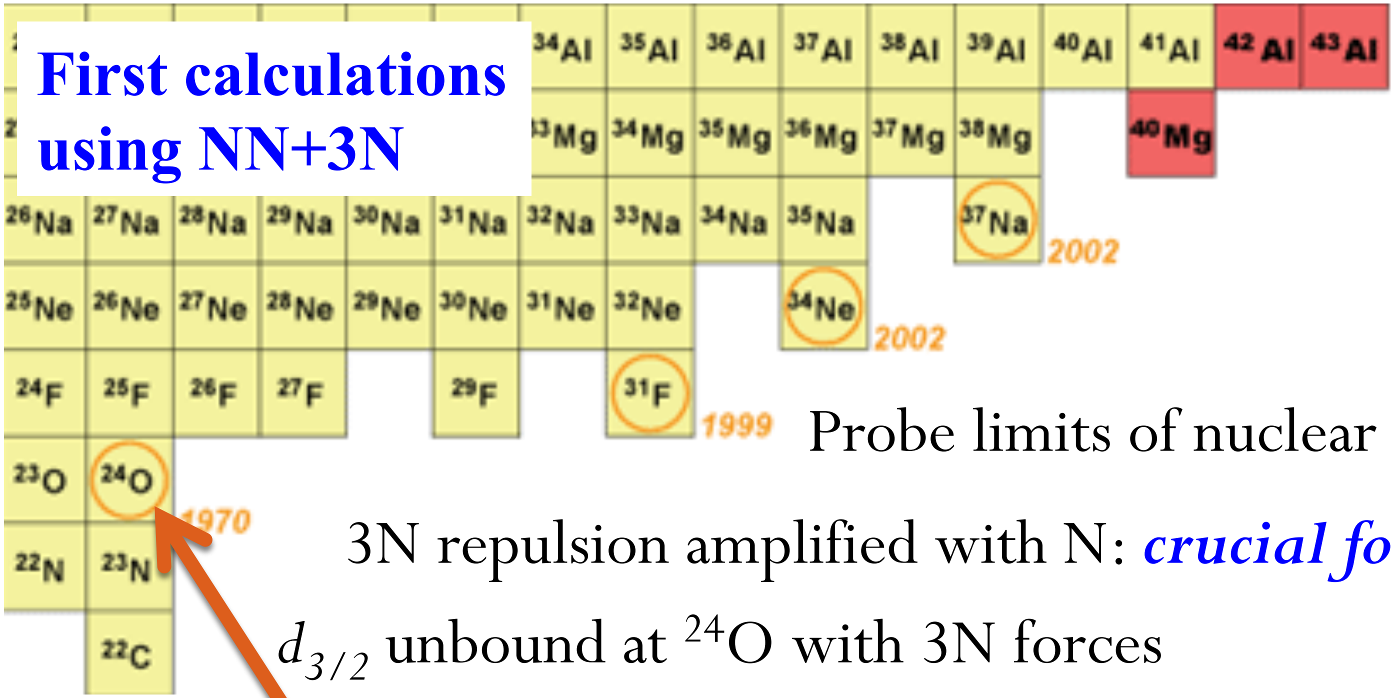
Effective two-body



$$\langle ab | \, V_{3N,\mathrm{eff}} \, | a'b' \rangle = \sum_{\alpha = core} \langle \alpha ab | \, V_{3N} \, | \alpha a'b' \rangle$$

Combine with NN (**Third Order**): no empirical adjustments

Oxygen Anomaly

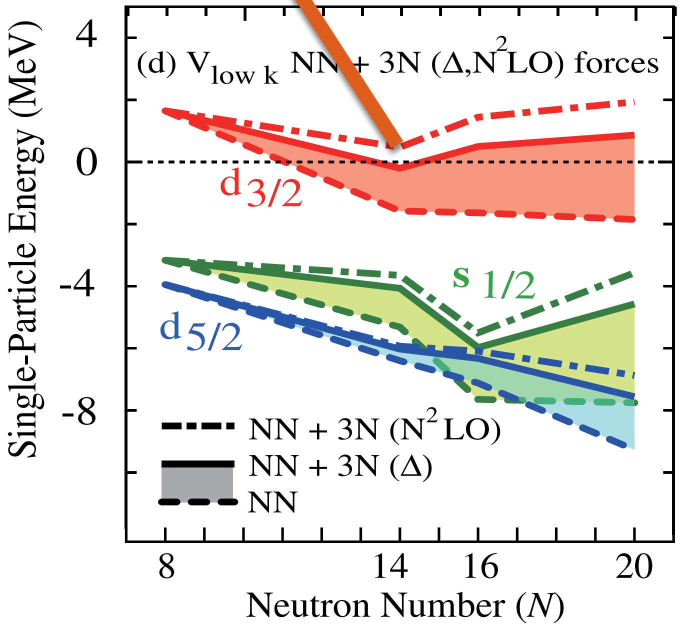


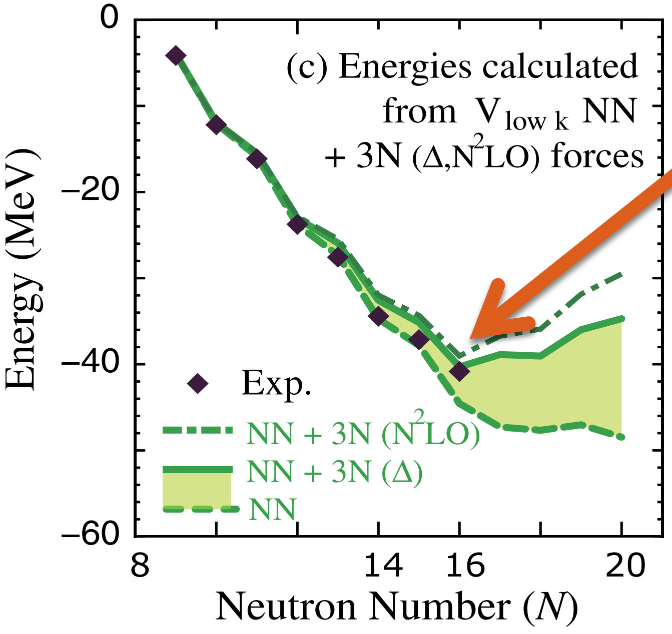
First calculations using NN+3N

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





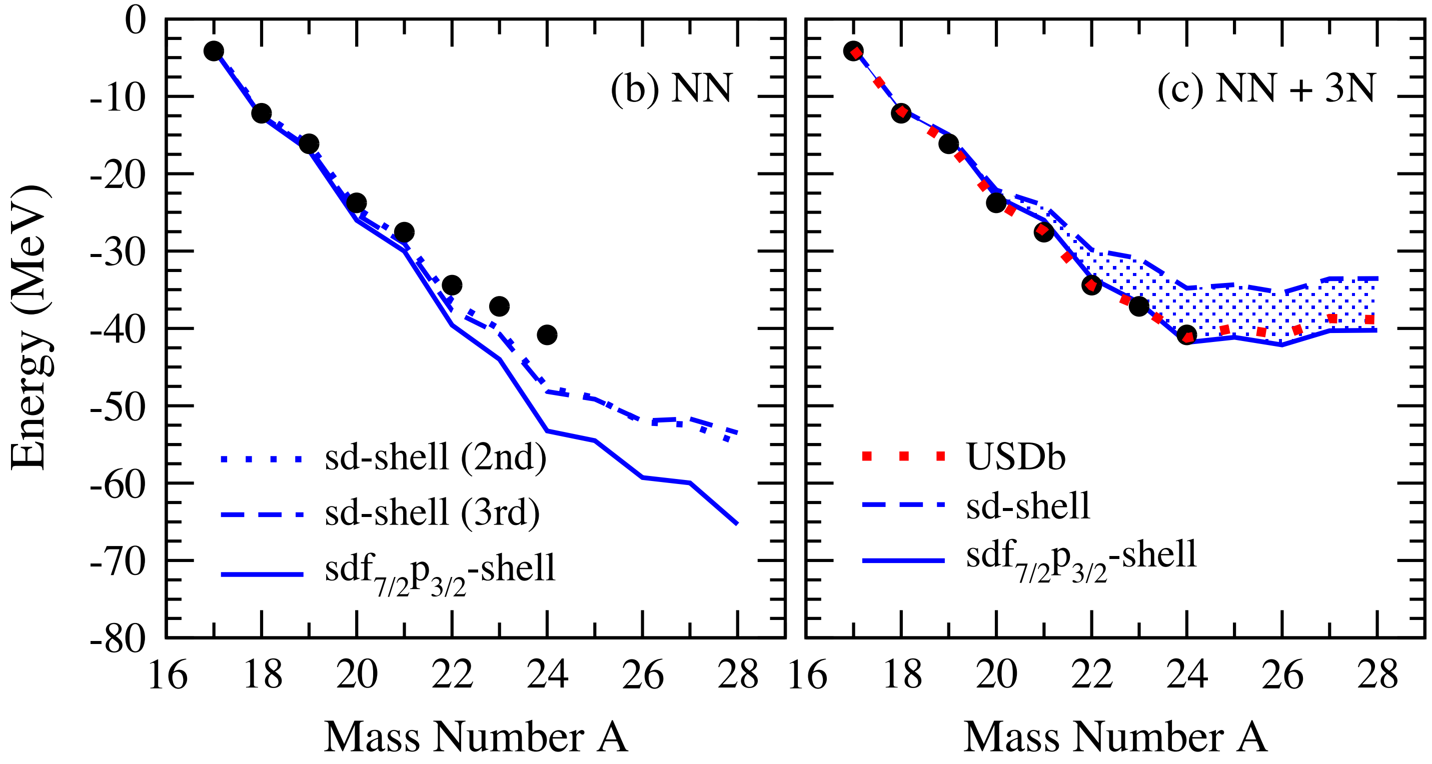
Isotopes unbound beyond ^{24}O

First microscopic explanation of oxygen anomaly

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

Ground-State Energies of Oxygen Isotopes

Valence-space interaction and SPEs from NN+3N



JDH, Menendez, Schwenk, EPJA (2013)

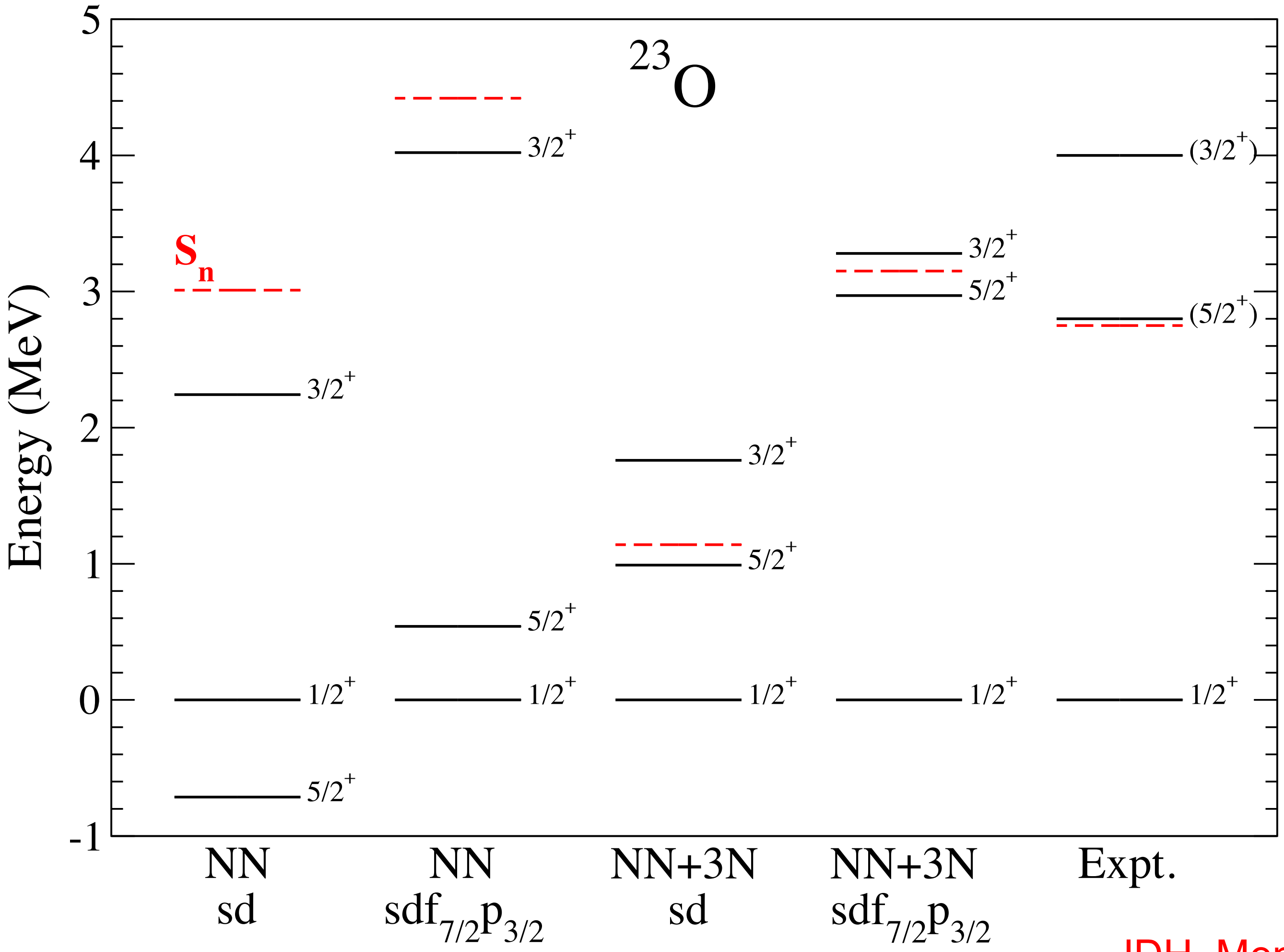
Repulsive character improves agreement with experiment

sd-shell results underbound; improved in **extended 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

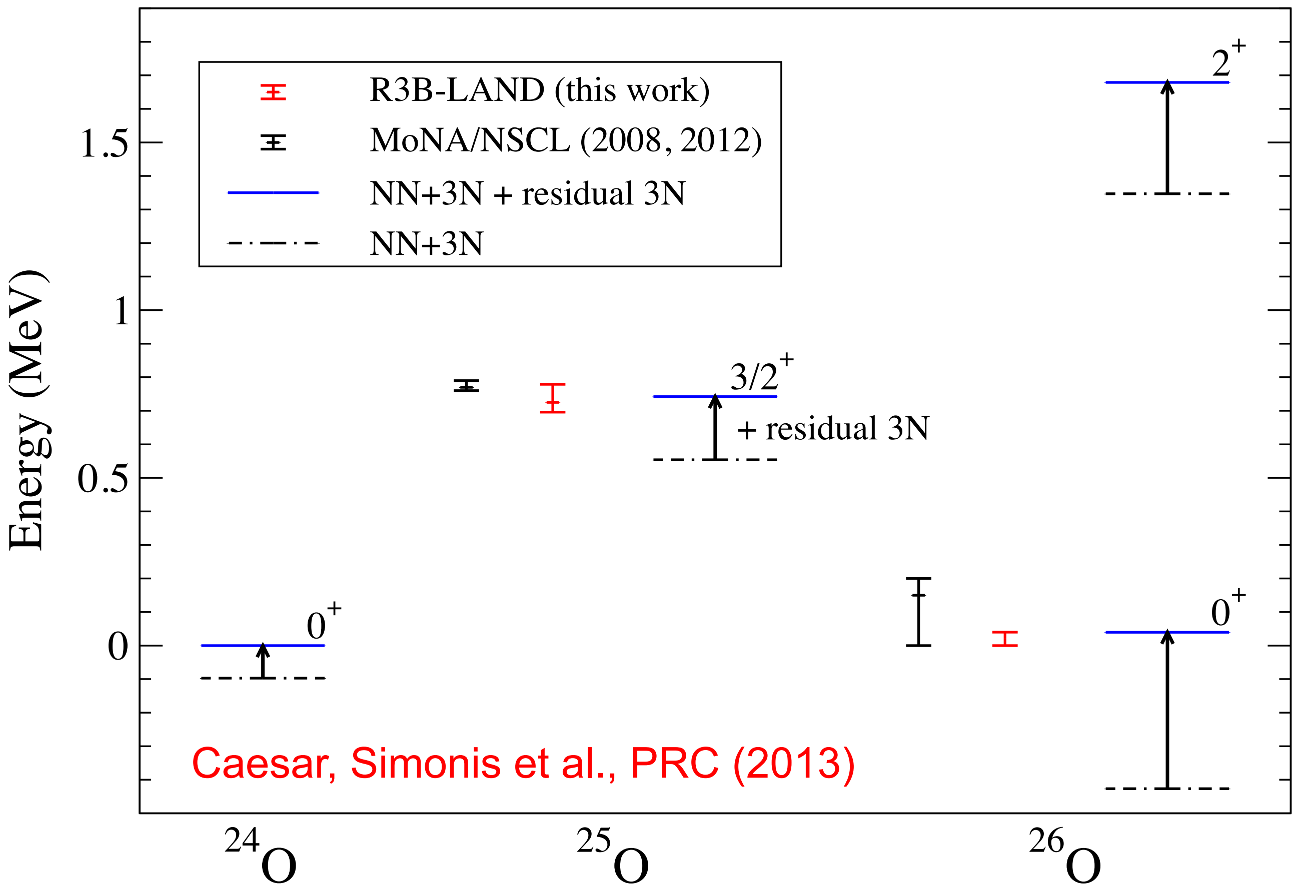
Clear improvement in extended valence space

JDH, Menendez, Schwenk, EPJA (2013)

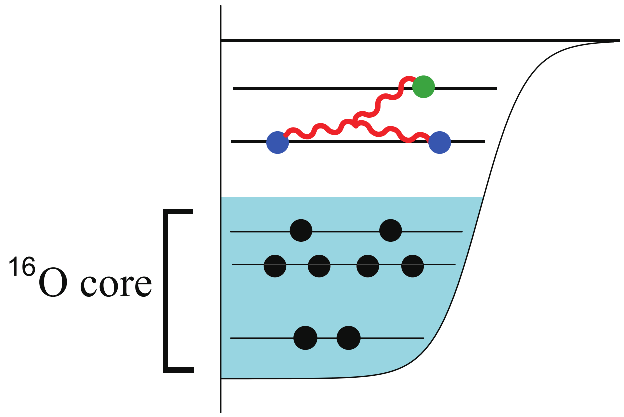
Experimental Connection: Beyond the Dripline

Hoffman, Kanungo, Lunderberg… PRLs (2008+)

Valence-space Hamiltonian from NN + 3N + **residual 3N**



Caesar, Simonis et al., PRC (2013)



	MBPT	Exp.
$S_n(^{25}O)$	742 keV	770 keV

	MBPT	Exp.
$S_{2n}(^{26}O)$	40 keV	<120 keV

Repulsion more pronounced for neutron-rich systems: 400 keV at ^{26}O

Improved agreement with new data beyond ^{24}O dripline

Future: include coupling to continuum

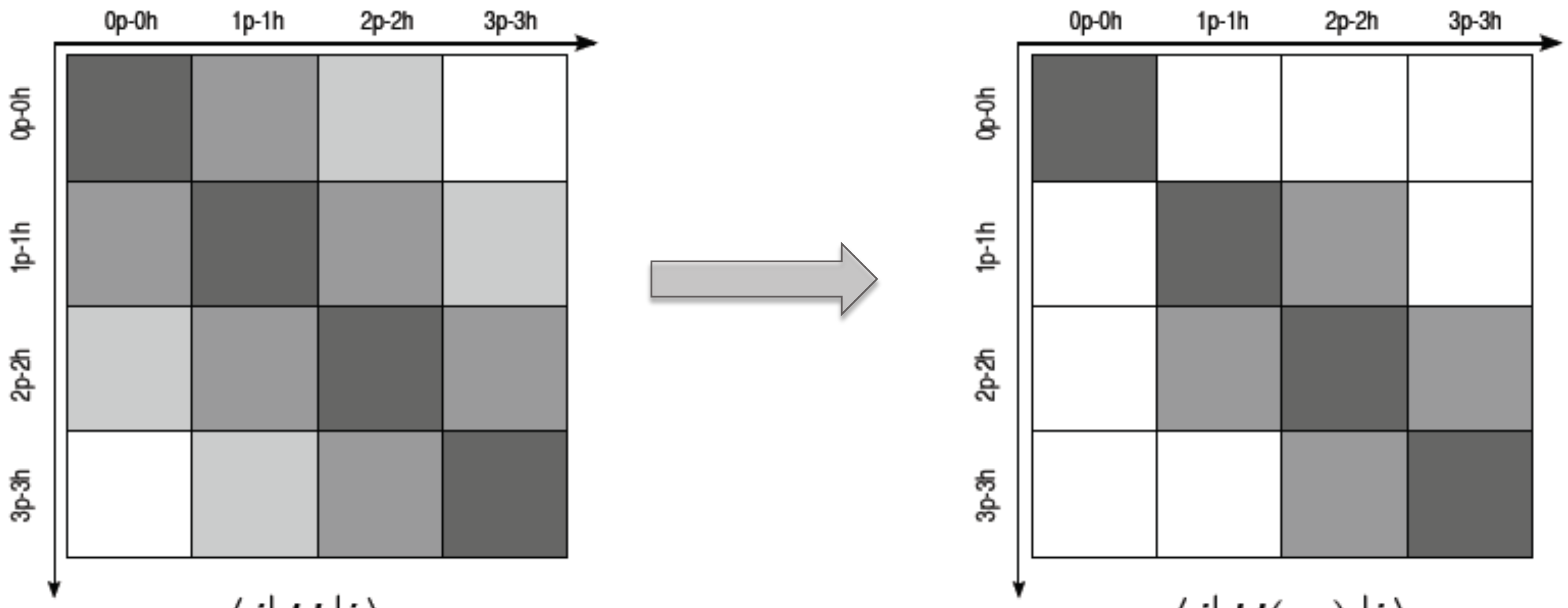
In-Medium SRG: Basics

In-Medium SRG applies continuous unitary transformation to drive off-diagonal physics to zero

Tsukiyama, Bogner, Schwenk, PRL (2011)

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

Decouples reference state from excitations $\langle npnh | H(\infty) | \Phi_c \rangle = 0$



$\langle i | H | j \rangle$ $\langle i | H(\infty) | j \rangle$

In-Medium SRG: Basics

In-Medium SRG applies continuous unitary transformation to drive off-diagonal physics to zero   Tsukiyama, Bogner, Schwenk, PRL (2011)

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

Where U is defined by the generator:

$$\eta(s) \equiv \left(\mathrm{d}U(s)/\mathrm{d}s\right)U^{\dagger}(s) \text{ chosen for desired decoupling behavior}$$

Taking

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

Drives H^{od} to 0 (Wegner, 1994)

Closed-shell reference state: drives all n-particle n-hole couplings to 0

$$\frac{\mathrm{d}H(s)}{\mathrm{d}s} = \left[\eta(s), H(s)\right] \qquad \left\langle npnh \middle| H(\infty) \middle| \Phi_c \right\rangle = 0$$

IM-SRG for Valence-Space Hamiltonians

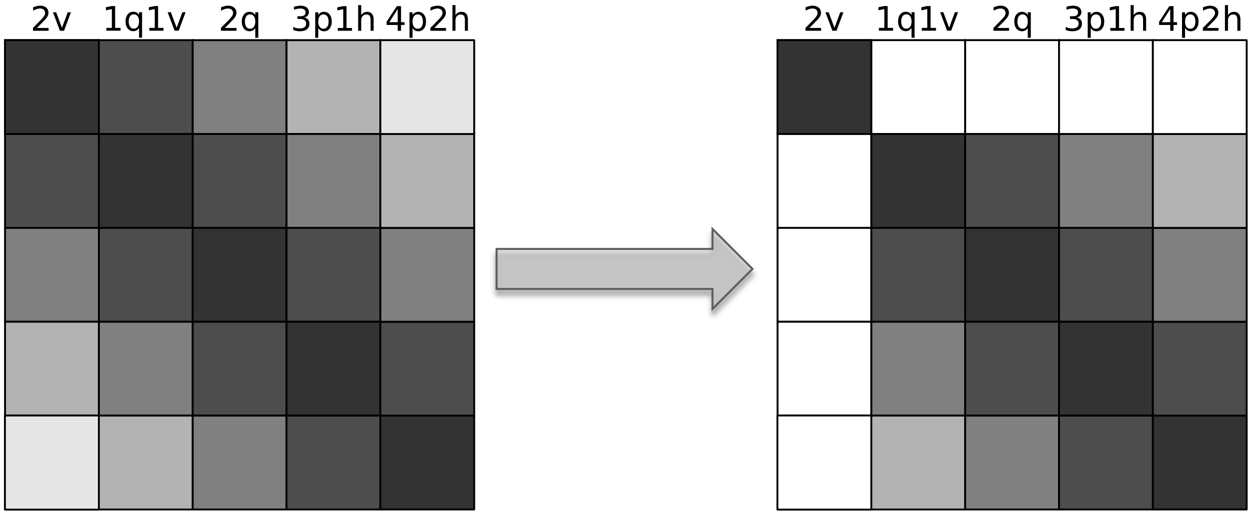
In-Medium SRG applies continuous unitary transformation to drive off-diagonal physics to zero

Tsukiyama, Bogner, Schwenk, PRC (2012)

Open shell systems:

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

Redefine "off-diagonal" to exclude valence particles



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

IM-SRG for Valence-Space Hamiltonians

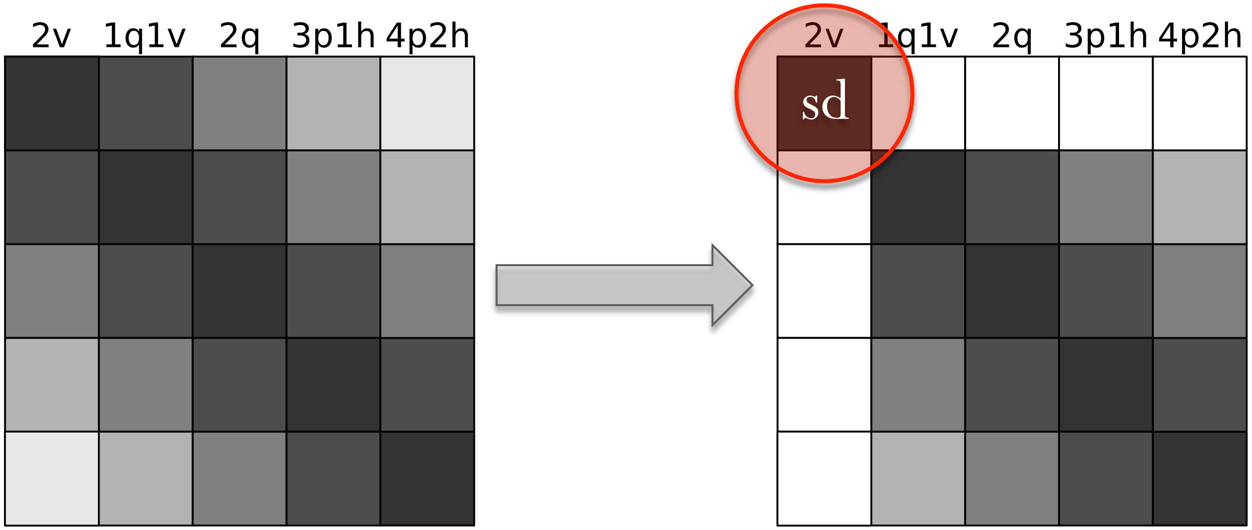
In-Medium SRG applies continuous unitary transformation to drive off-diagonal physics to zero

Tsukiyama, Bogner, Schwenk, PRC (2012)

Open shell systems:

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

Redefine "off-diagonal" to exclude valence particles



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

Defines new effective valence-space Hamiltonian H_{eff}

States outside valence space are decoupled

Nonperturbative Valence-Space Strategy

1) Effective interaction: nonperturbative from IM-SRG

2) Single-particle energies: nonperturbative from IM-SRG

3) Hartree-Fock basis of $e_{\max} = 2n + l = 14$ **converged**

★4) NN and 3N forces from chiral EFT

5) Explore extended valence spaces – in progress

NN matrix elements

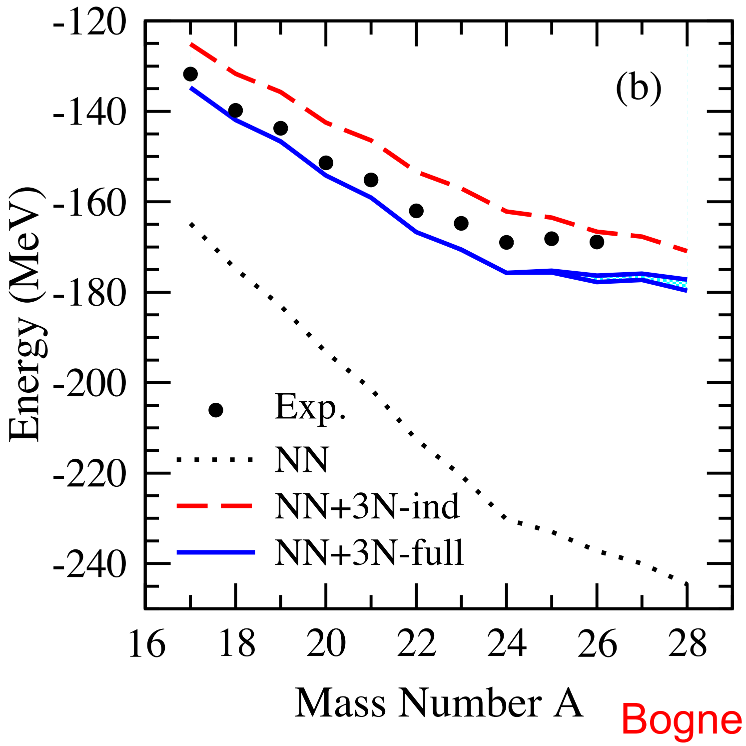
- Chiral N^{3}LO (Machleidt, $\Lambda_{NN} = 500\text{MeV}$); free-space SRG evolution
- Cutoff variation $\lambda_{SRG} = 1.88 - 2.24\text{fm}^{-1}$
- Vary $\hbar\omega = 20 - 24\text{MeV}$
- Consistently include 3N forces induced by SRG evolution (**NN+3N-ind**)

Initial 3N force contributions

- Chiral N^{2}LO $\Lambda_{3N} = 400\text{MeV}$ (**NN+3N-full**)
- Included with cut: $e_1 + e_2 + e_3 \leq E_{3\max} = 14$

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

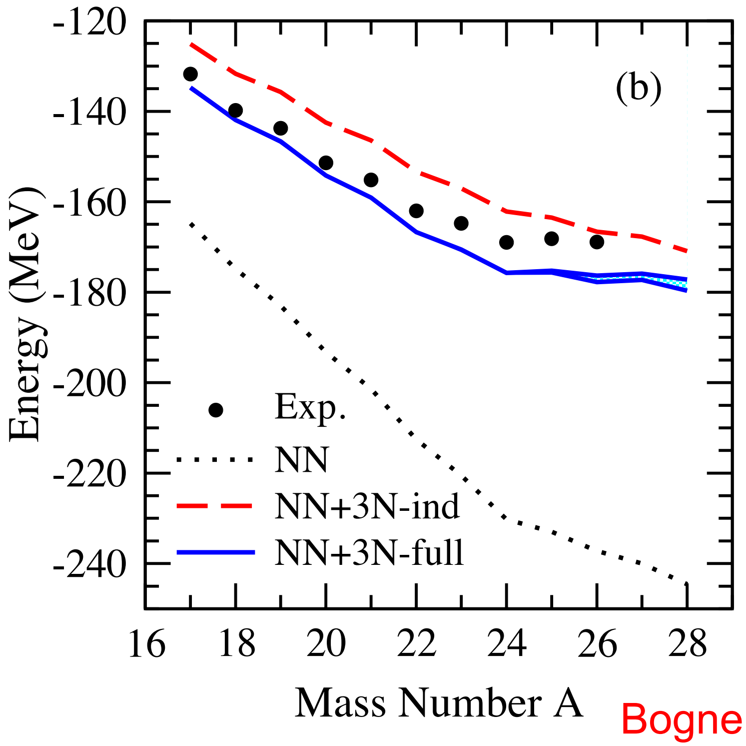
NN+3N-full modestly overbound – good behavior past dripline

Good dripline properties

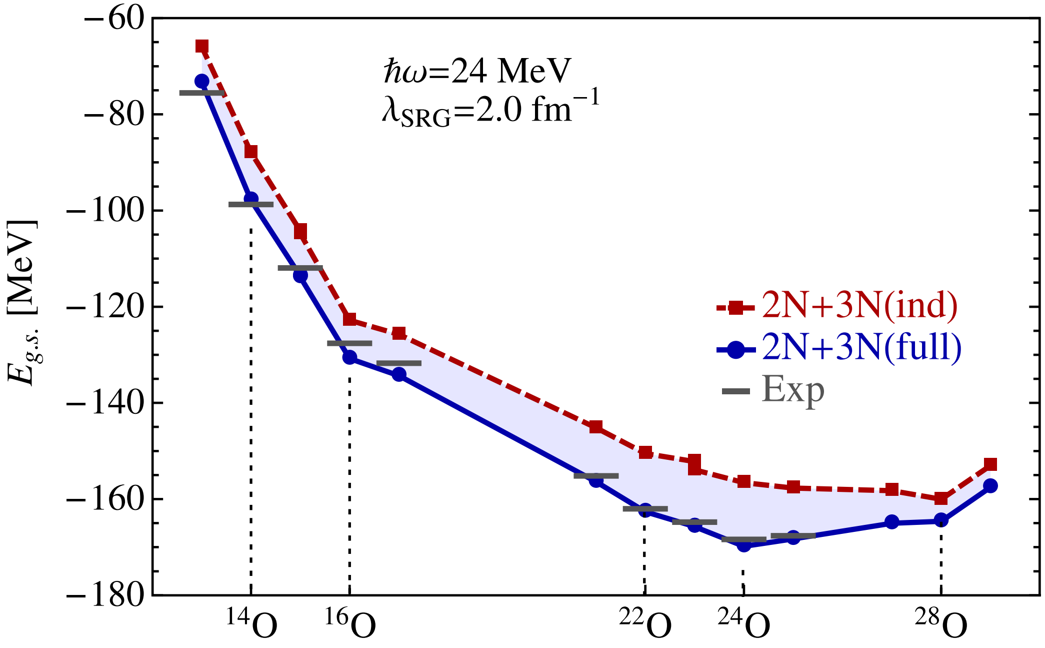
Very weak $\hbar\omega$ dependence

IM-SRG Oxygen Ground-State Energies

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



Bogner et al., PRL (2014)



Cipollone, Barbieri, Navratil, PRL (2013)

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

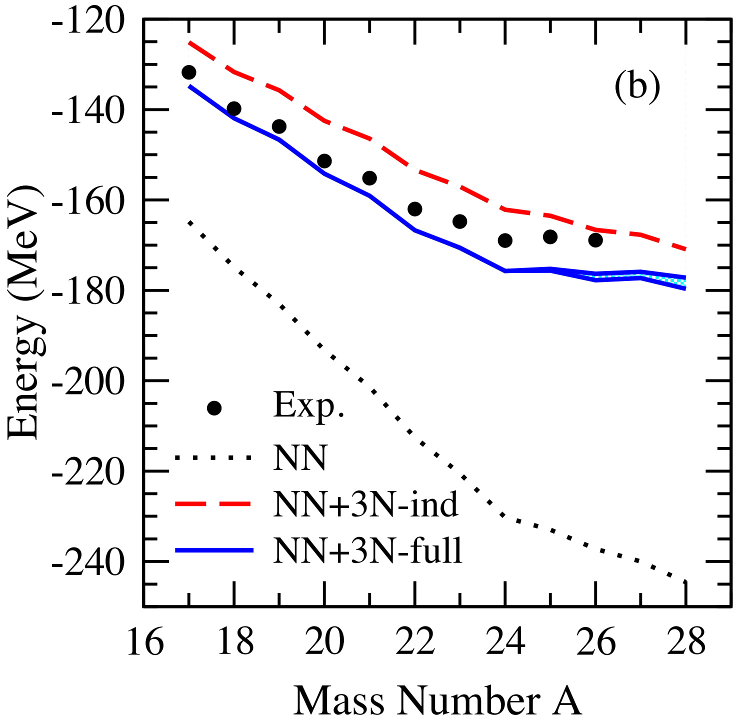
NN+3N-full modestly overbound – good behavior past dripline

Good dripline properties

Very weak $\hbar\omega$ dependence

Comparison with Large-Space Methods

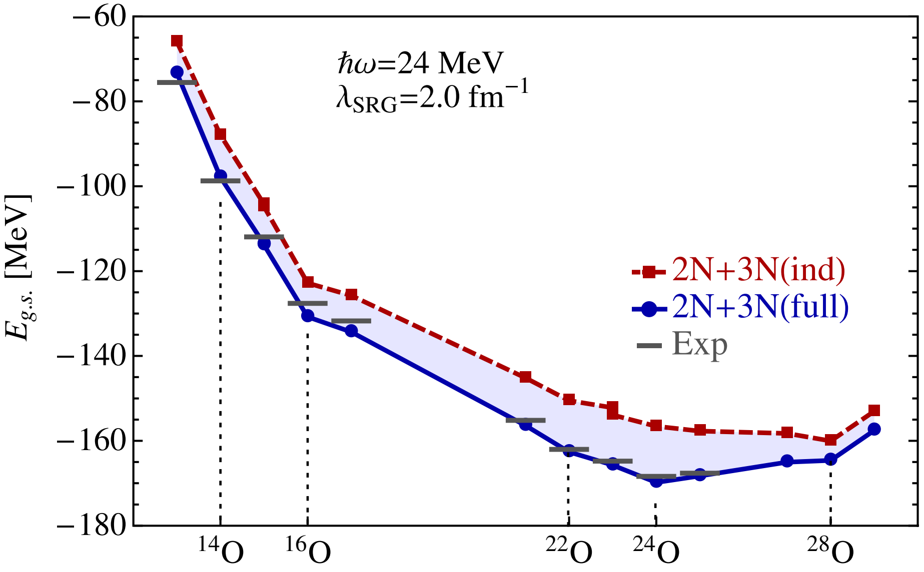
Large-space methods with same SRG-evolved NN+3N forces



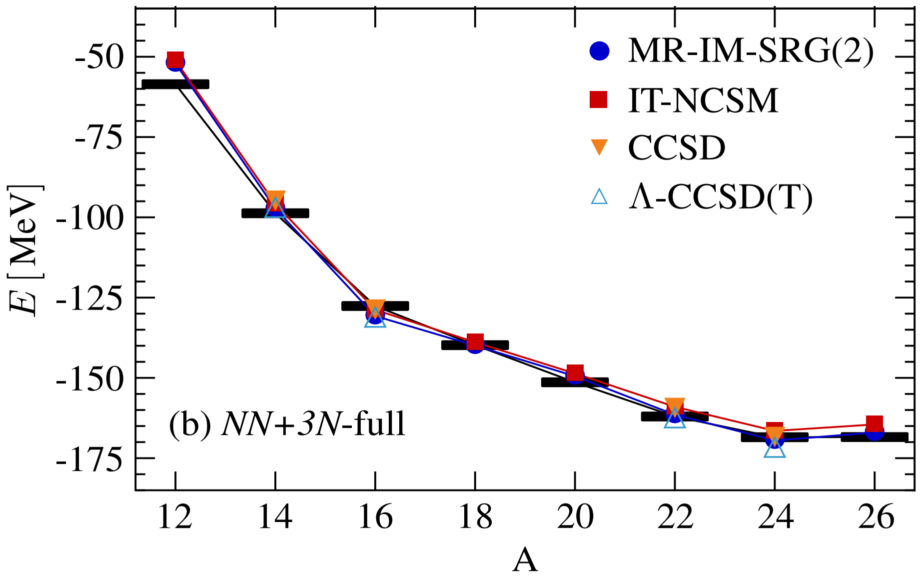
Clear improvement with full NN+3N

Confirms valence-space results

Remarkable agreement with same forces



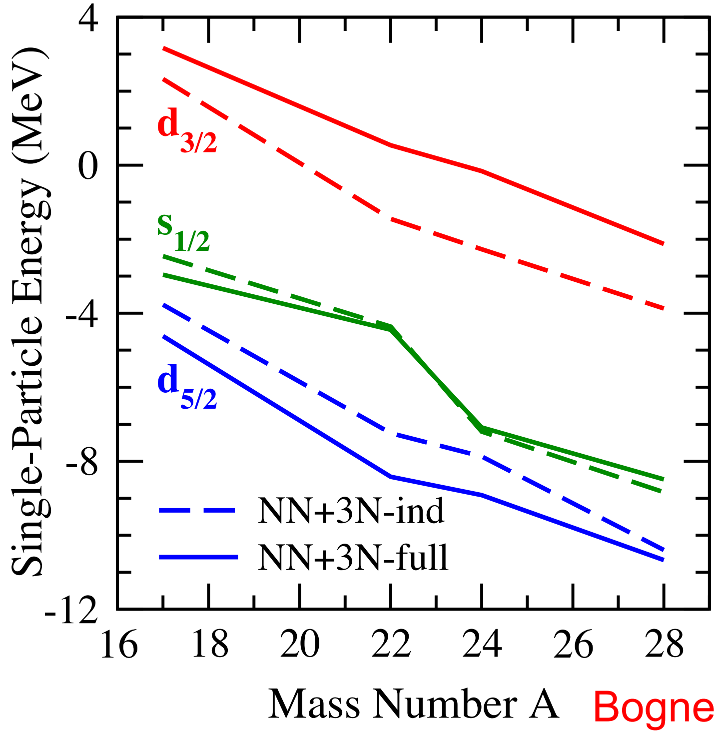
Cipollone, Barbieri, Navratil, PRL (2013)



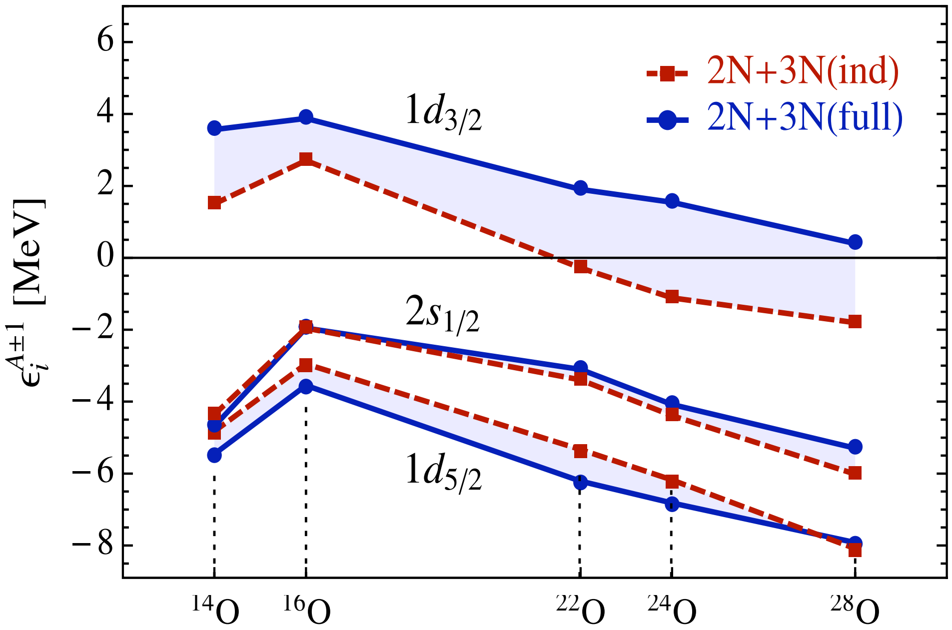
Hergert et al., PRL (2013)

Dripline Mechanism

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



Bogner et al., PRL (2014)



Cipollone, Barbieri, Navratil, PRL (2013)

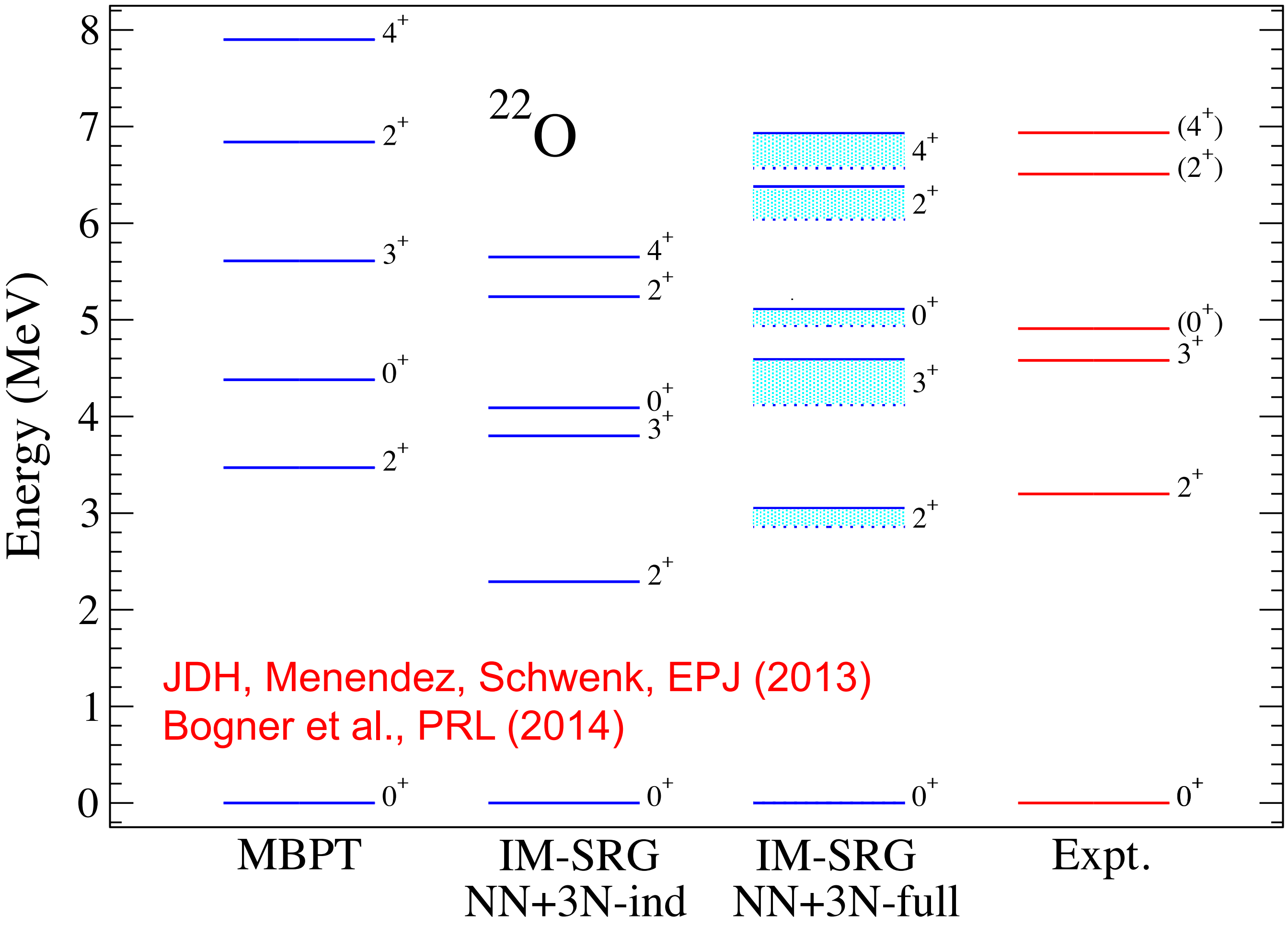
Robust mechanism driving dripline behavior

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

Similar to initial MBPT NN+3N calculations in oxygen

IM-SRG Oxygen Spectra

Oxygen spectra: extended-space MBPT and IM-SRG

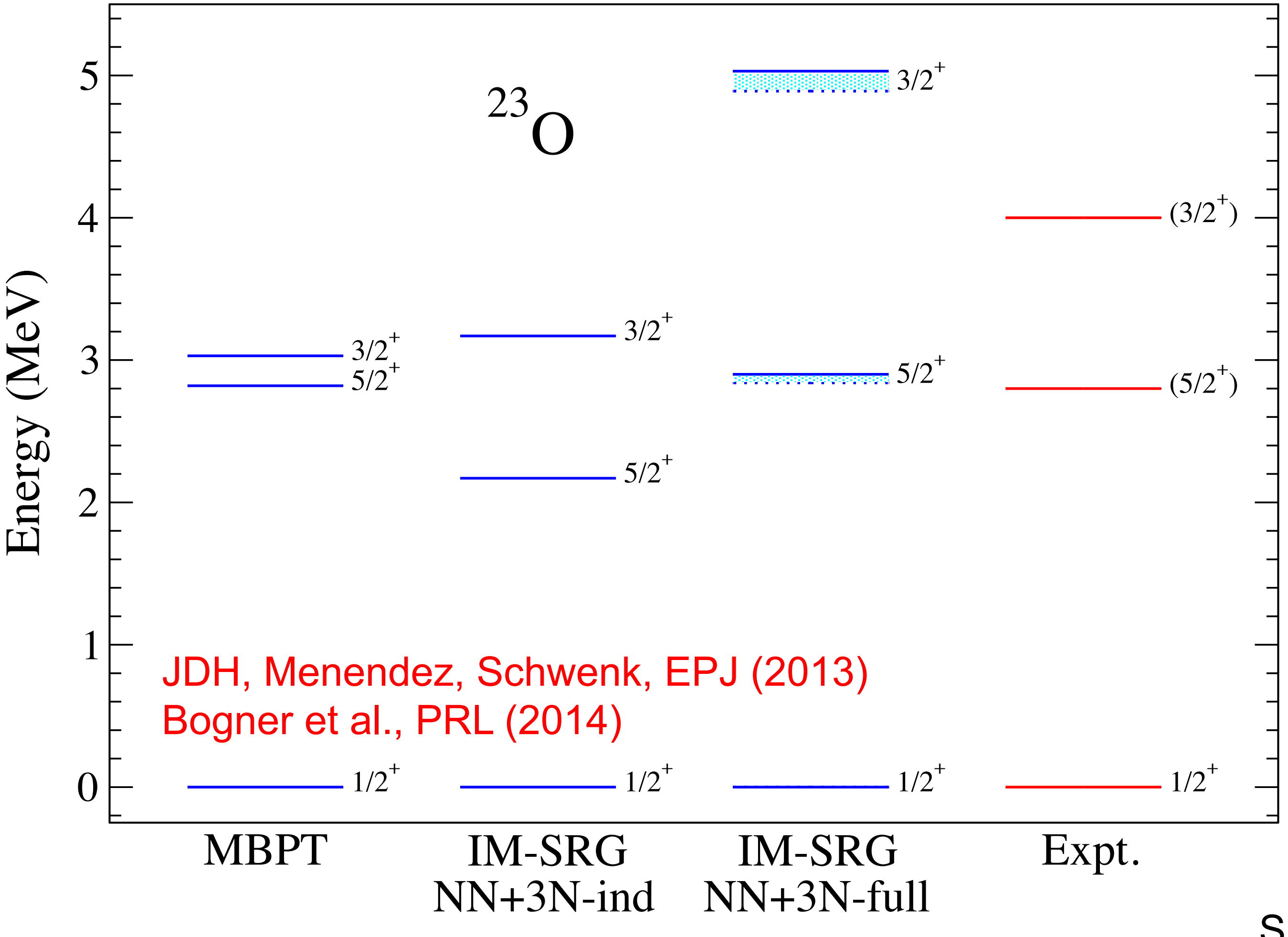


Clear improvement with NN+3N-full

IM-SRG: comparable with phenomenology

IM-SRG Oxygen Spectra

Oxygen spectra: extended-space MBPT and IM-SRG



JDH, Menendez, Schwenk, EPJ (2013)
Bogner et al., PRL (2014)

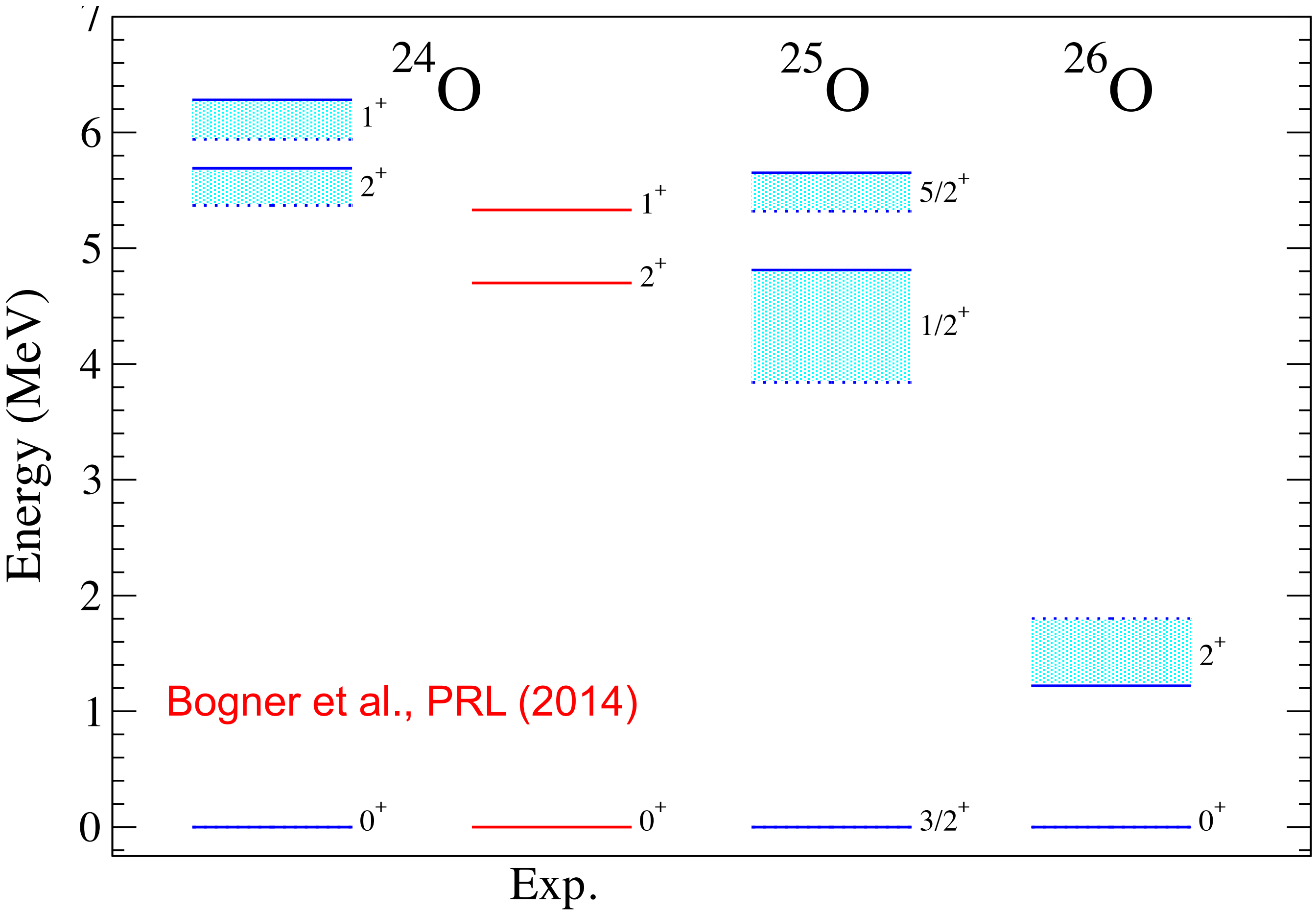
Similar CC valence-space results:
G. Jansen et al., arXiv:1402.2563

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



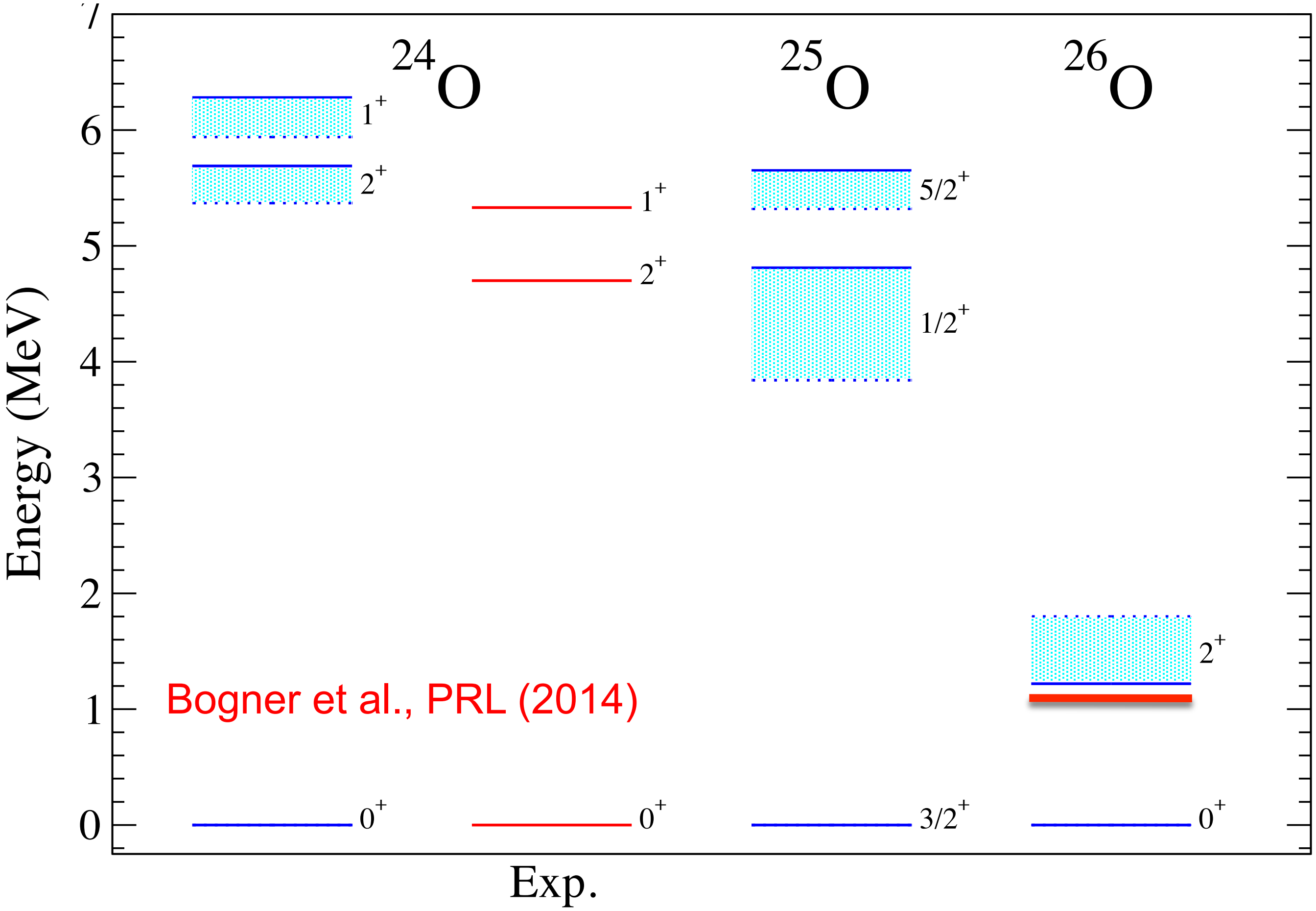
^{24}O closed shell (too high 2^+)

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



Bogner et al., PRL (2014)

Kondo et al., PRELIMINARY

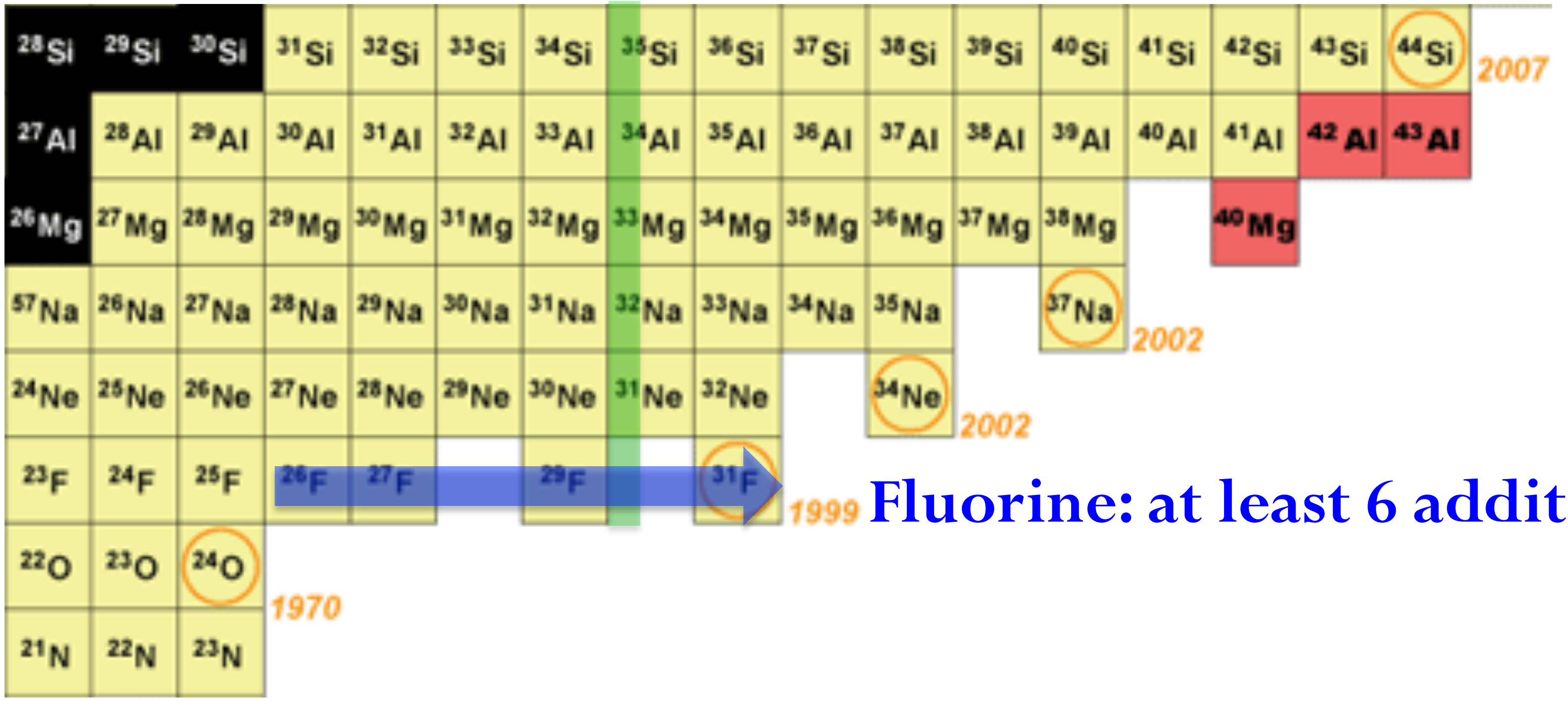
New measurement at RIKEN on excited states in ^{26}O

Existence of excited state "just over 1.0 MeV" (uncertainty not finalized)

Towards Full sd-Shell with MBPT: Fluorine

Next challenge: **valence protons + neutrons**

Neutron-rich fluorine and neon



Fluorine: at least 6 additional neutrons

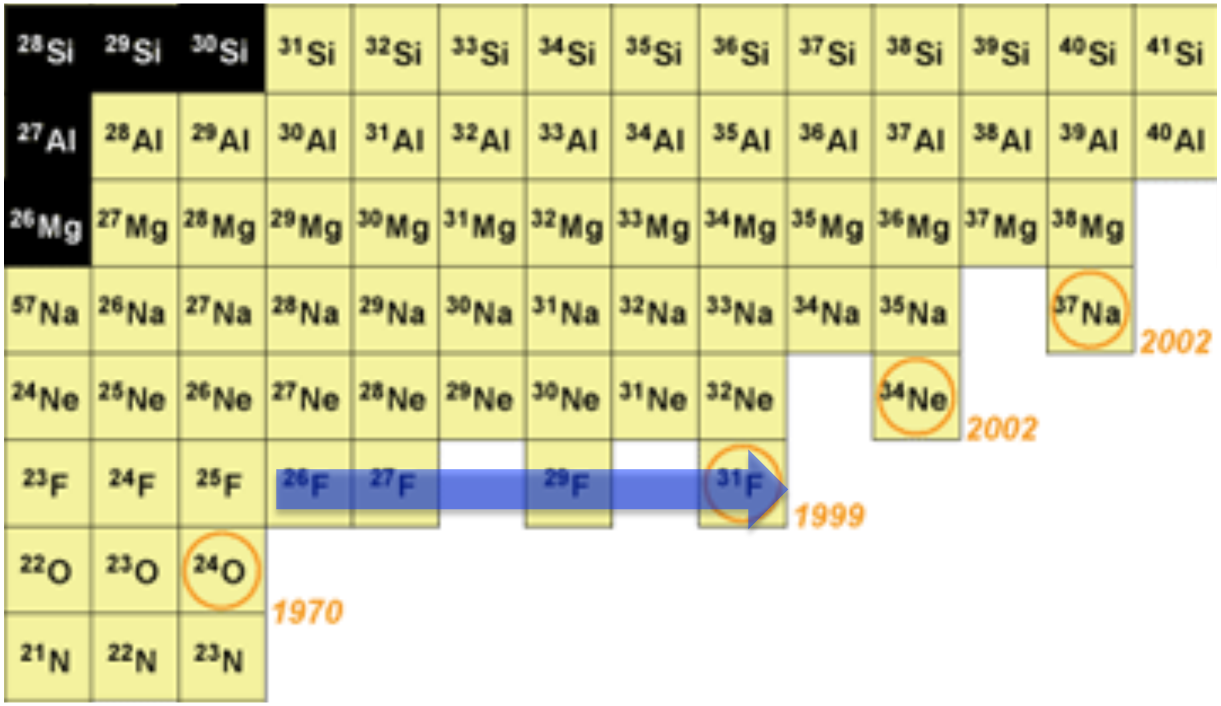
sd shell filled at ^{29}F/^{30}Ne

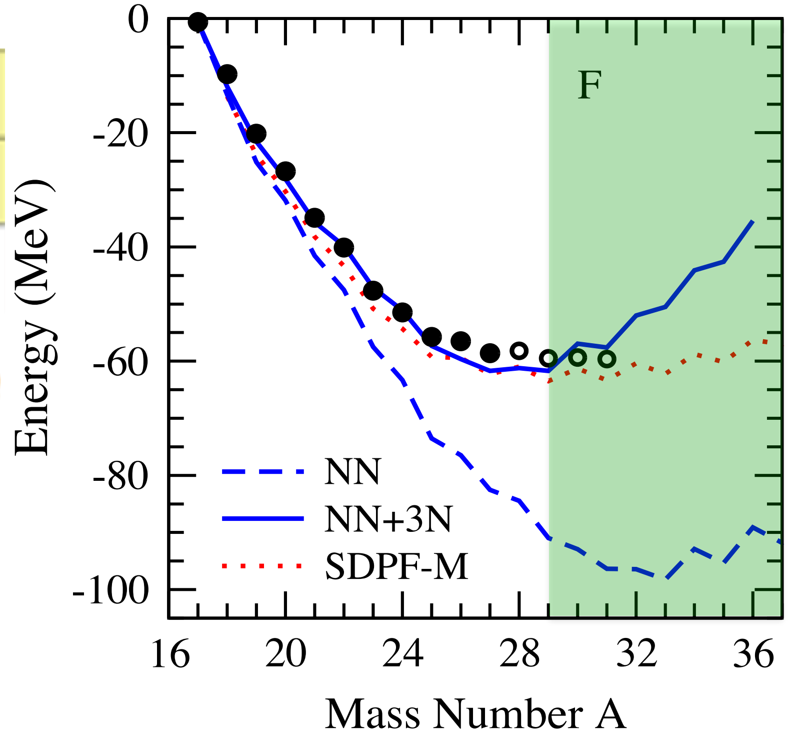
Need extended-space orbits

Towards Full sd-Shell with MBPT: Fluorine

Next challenge: **valence protons + neutrons**

Neutron-rich fluorine and neon





JDH, Menendez, Simonis, Schwenk, in prep.

NN only: severe overbinding

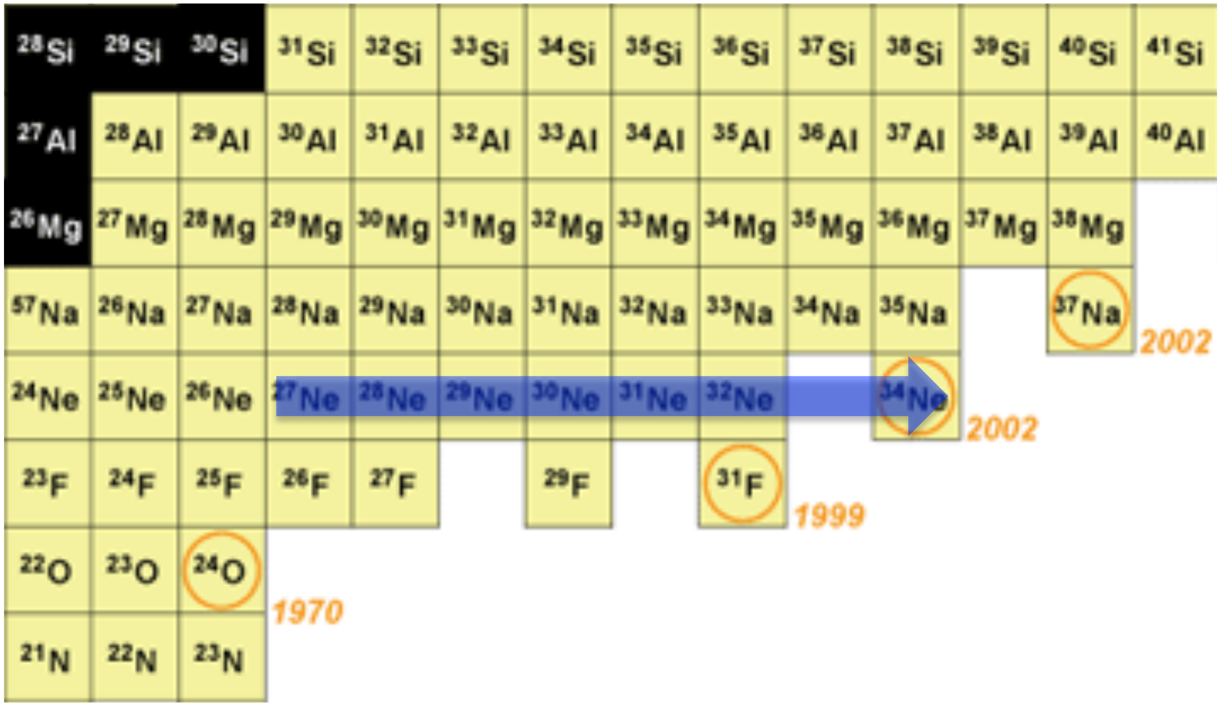
NN+3N: good experimental agreement through ^{29}F

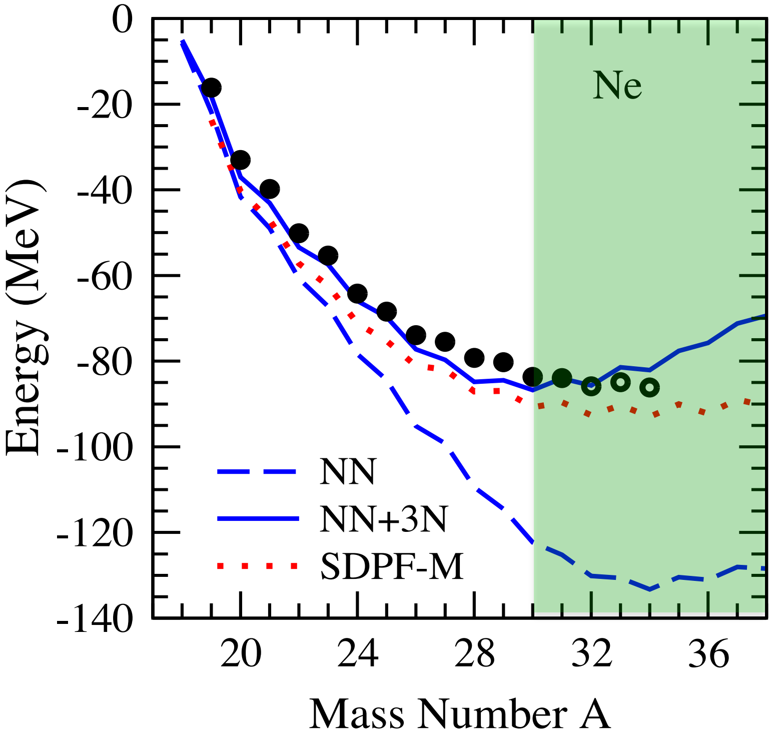
Sharp increase in ground-state energies beyond ^{29}F: incorrect dripline

Towards Full sd-Shell with MBPT: Neon

Next challenge: **valence protons + neutrons**

Neutron-rich fluorine and neon





JDH, Menendez, Simonis, Schwenk, in prep.

Similar behavior in Neon isotopes

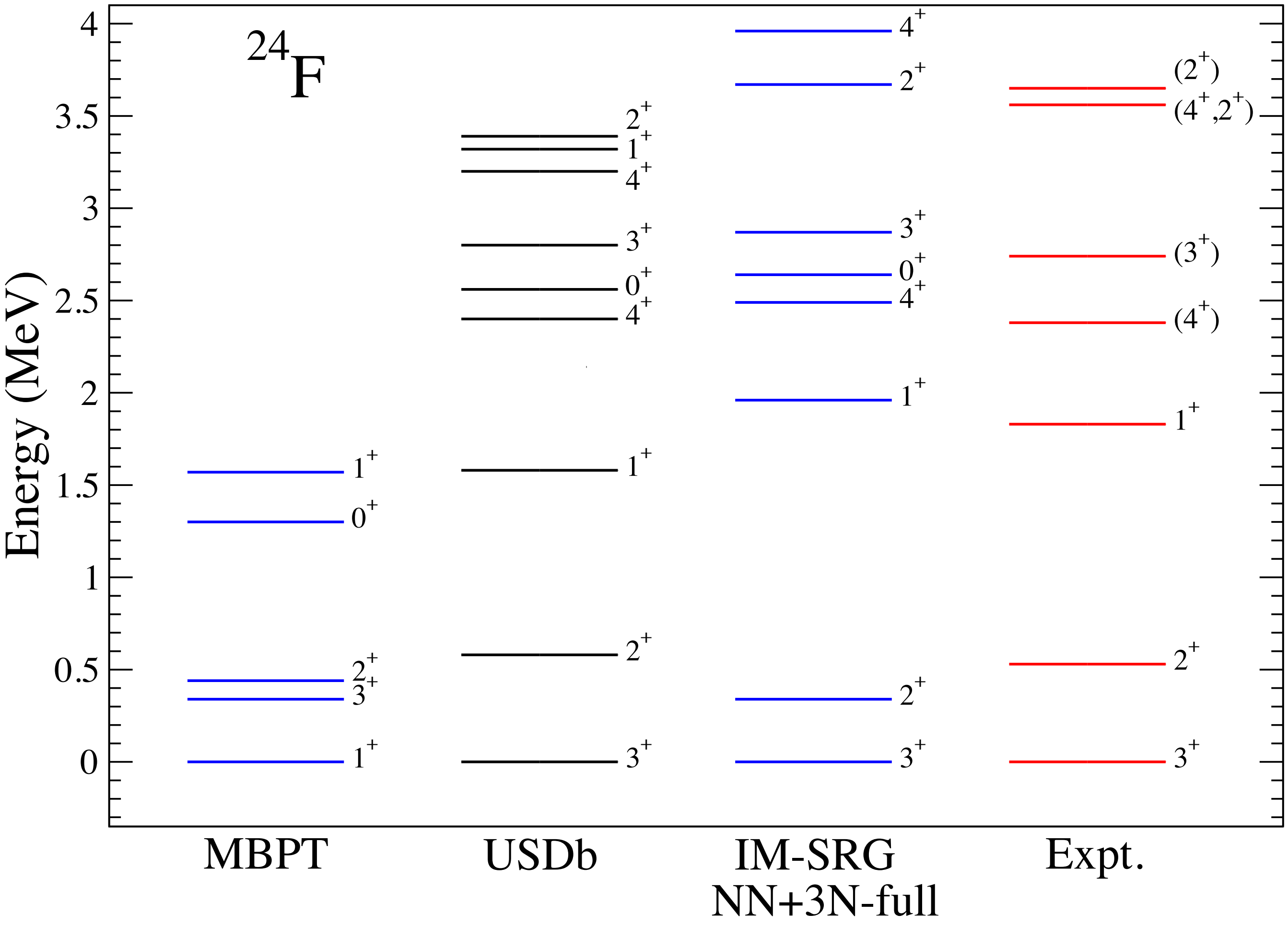
Revisit cross-shell valence space theory – **non-degenerate valence spaces**

Tsunoda, Hjorth-Jensen, Otsuka

IM-SRG energies overbound in F/Ne

Experimental Connection: ^{24}F Spectrum

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



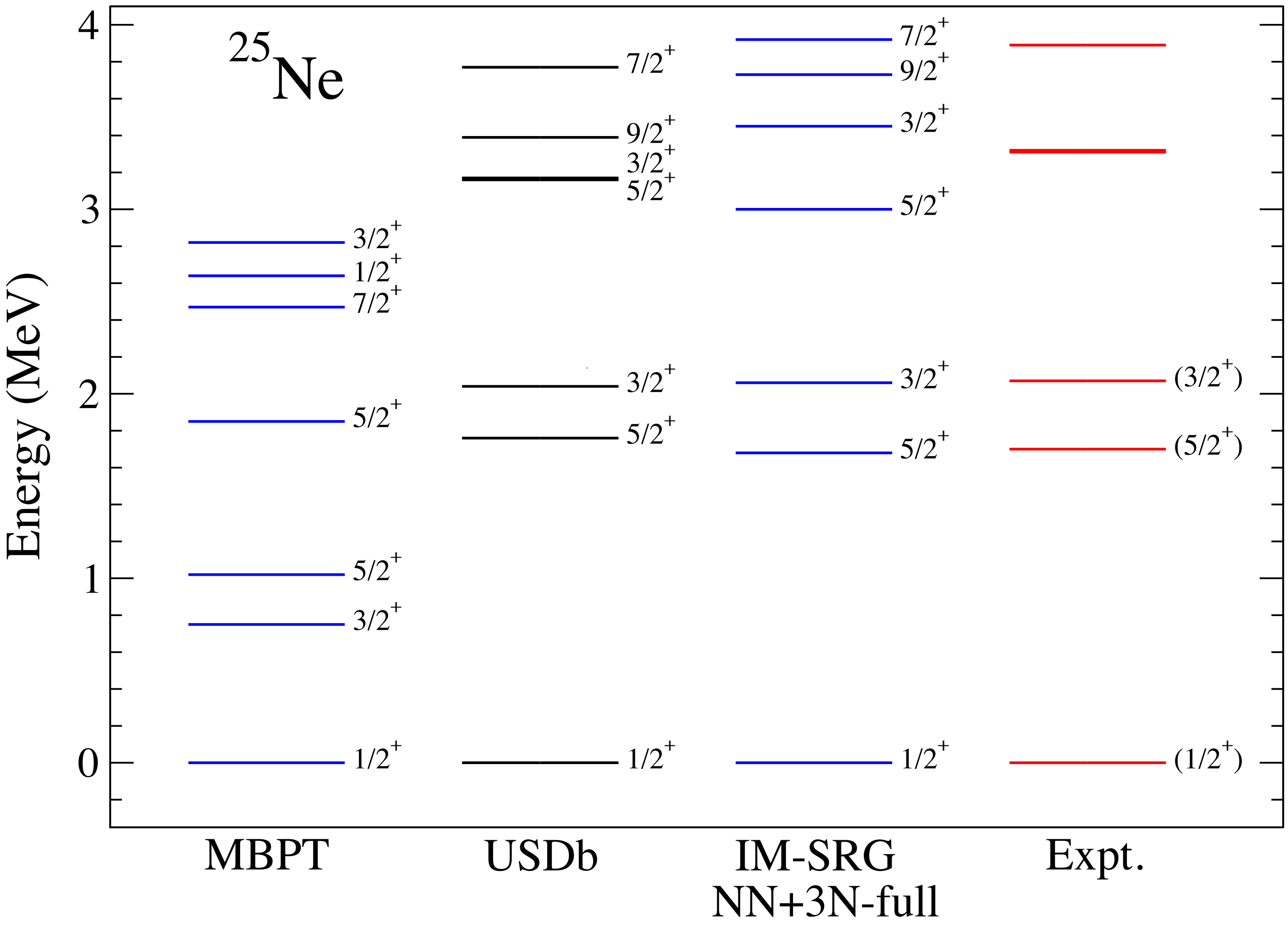
Caceres et al., in prep.

New measurements from GANIL

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

^{25}Ne Spectrum

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



Bogner, Hergert, JDH, Schwenk, in prep

Limited experimental data

IM-SRG: comparable with phenomenology, good agreement with data

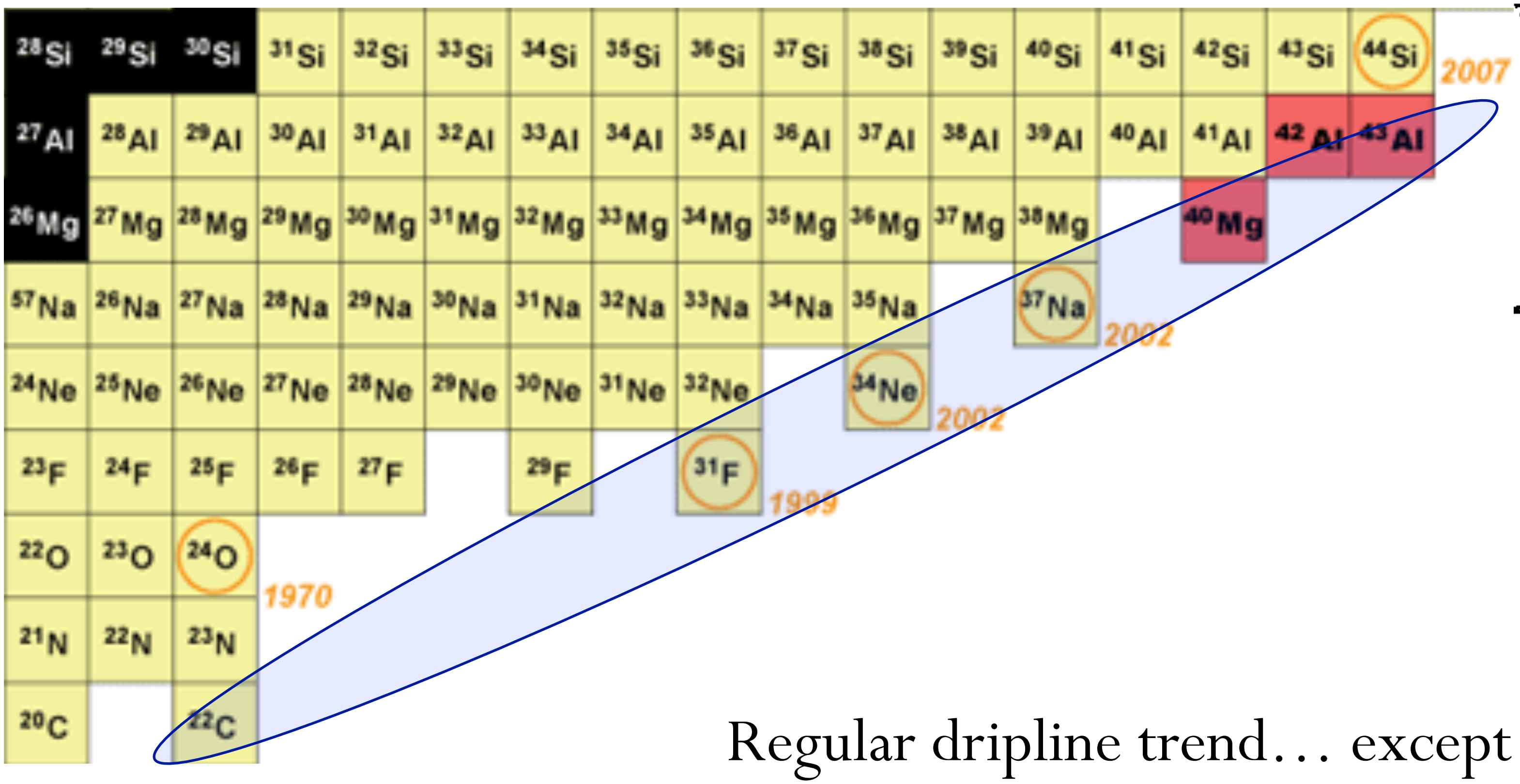
Limits of Nuclear Existence: Oxygen Anomaly

Where is the nuclear dripline?

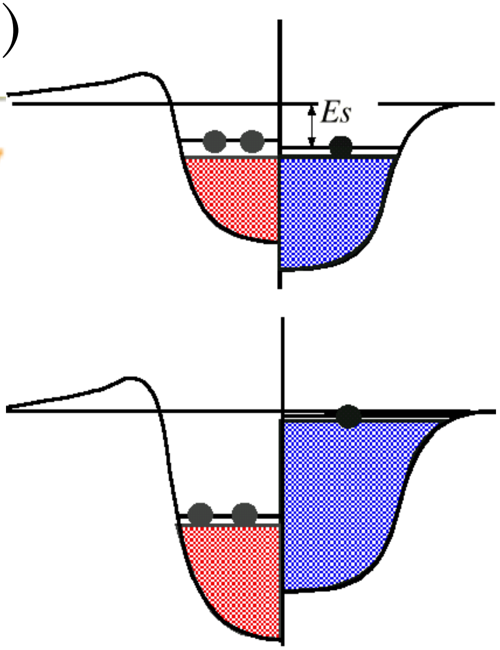
Limits defined as last isotope with positive neutron separation energy

- Nucleons "drip" out of nucleus

Neutron dripline experimentally established to Z=8 (Oxygen)



^{28}Si	^{29}Si	^{30}Si	^{31}Si	^{32}Si	^{33}Si	^{34}Si	^{35}Si	^{36}Si	^{37}Si	^{38}Si	^{39}Si	^{40}Si	^{41}Si	^{42}Si	^{43}Si	^{44}Si	2007
^{27}Al	^{28}Al	^{29}Al	^{30}Al	^{31}Al	^{32}Al	^{33}Al	^{34}Al	^{35}Al	^{36}Al	^{37}Al	^{38}Al	^{39}Al	^{40}Al	^{41}Al	^{42}Al	^{43}Al	
^{26}Mg	^{27}Mg	^{28}Mg	^{29}Mg	^{30}Mg	^{31}Mg	^{32}Mg	^{33}Mg	^{34}Mg	^{35}Mg	^{36}Mg	^{37}Mg	^{38}Mg		^{40}Mg			
^{25}Na	^{26}Na	^{27}Na	^{28}Na	^{29}Na	^{30}Na	^{31}Na	^{32}Na	^{33}Na	^{34}Na	^{35}Na		^{37}Na					
^{24}Ne	^{25}Ne	^{26}Ne	^{27}Ne	^{28}Ne	^{29}Ne	^{30}Ne	^{31}Ne	^{32}Ne		^{34}Ne			2002				
^{23}F	^{24}F	^{25}F	^{26}F	^{27}F		^{29}F		^{31}F			2002						
^{22}O	^{23}O	^{24}O							1999								
^{21}N	^{22}N	^{23}N	1970														
^{20}C		^{22}C															

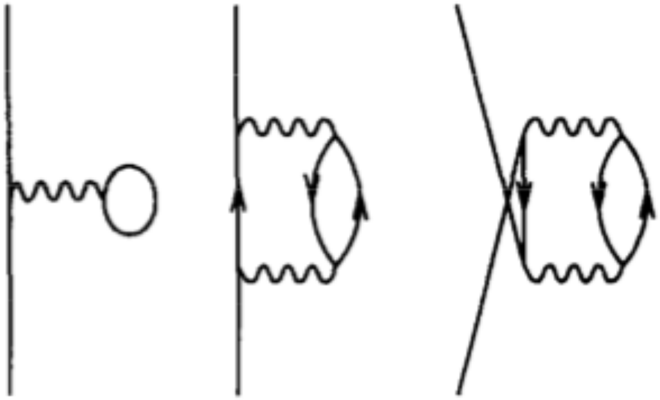


Regular dripline trend… except anomalous oxygen

Adding one proton binds 6 additional neutrons

Single Particle Energies

SPEs **self-consistently** from one-body diagrams



+ 3rd order

sd-shell: overbound, unreasonable spacing

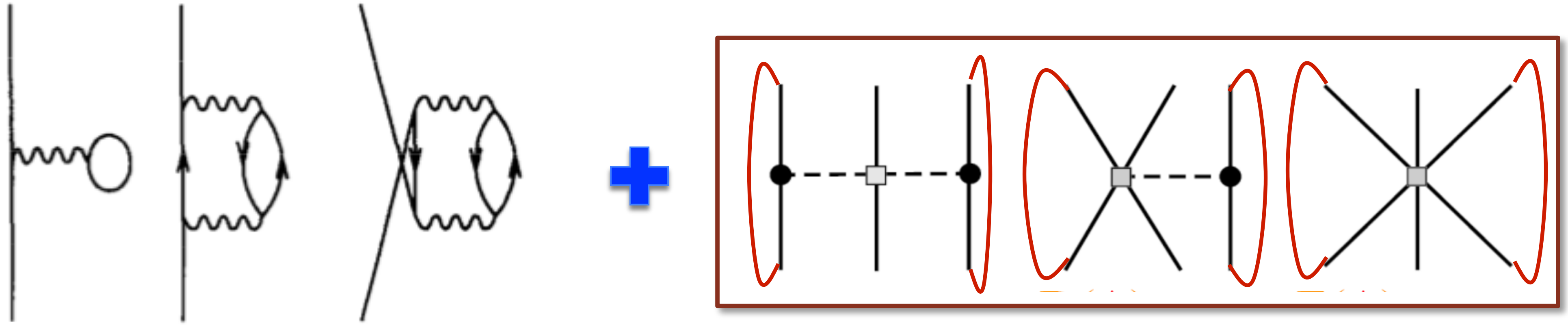
Orbit	"Exp"	USDb	$T+V_{NN}$ (3rd)
$d_{5/2}$	-4.14	-3.93	**-5.43**
$s_{1/2}$	-3.27	-3.21	**-5.32**
$d_{3/2}$	0.944	2.11	**-0.97**

Typical approach: use empirical SPEs

3N forces eliminate need for adjusted parameters?

One-Body 3N: Single Particle Energies

NN-only microscopic SPEs yield poor results – rely on empirical adjustments



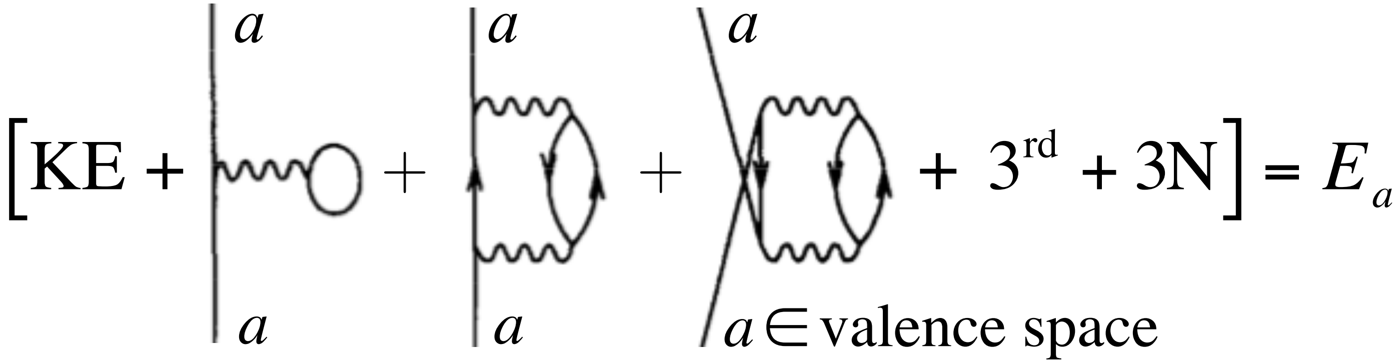
sd-shell: SPEs much too bound, unreasonable splitting

3N forces: additional repulsion – comparable to phenomenology

Orbit	**USDb**	$T+V_{NN}+V_{3N}$
$d_{5/2}$	-3.93	-3.78
$s_{1/2}$	-3.21	-2.42
$d_{3/2}$	2.11	1.45

Single-Particle Energies with NN+3N Forces

3N forces: additional repulsion improves SPEs



Orbit *a*	**USDb**	**$T+V_{NN}$**	**$T+V_{NN}+V_{3N}$**	**SDPF-M**	**$T+V_{NN}+V_{3N}$**
$d_{5/2}$	-3.93	-5.43	**-3.78**	-3.95	**-3.46**
$s_{1/2}$	-3.21	-5.32	**-2.42**	-3.16	**-2.20**
$d_{3/2}$	2.11	-0.97	**1.45**	1.65	**1.92**
$f_{7/2}$				3.10	**3.71**
$p_{3/2}$				3.10	**7.72**

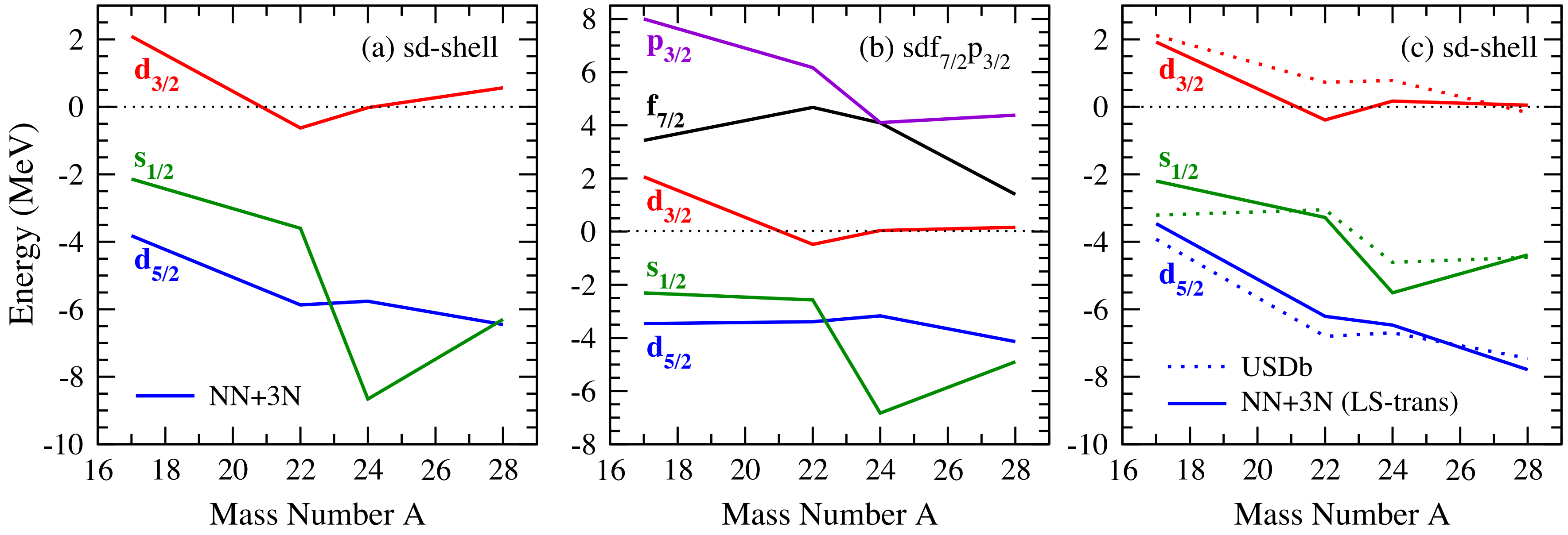
JDH, Menendez, Schwenk, EPJA (2013)

Similar contributions in standard/extended valence spaces

Comparable with phenomenology

Non-Observability of Shell Gaps

SPE evolution with 3N forces in *sd* and $sdf_{7/2}p_{3/2}$ spaces:



Duguet, Hergert, JDH, Soma, in prep.

NN+3N extended space:

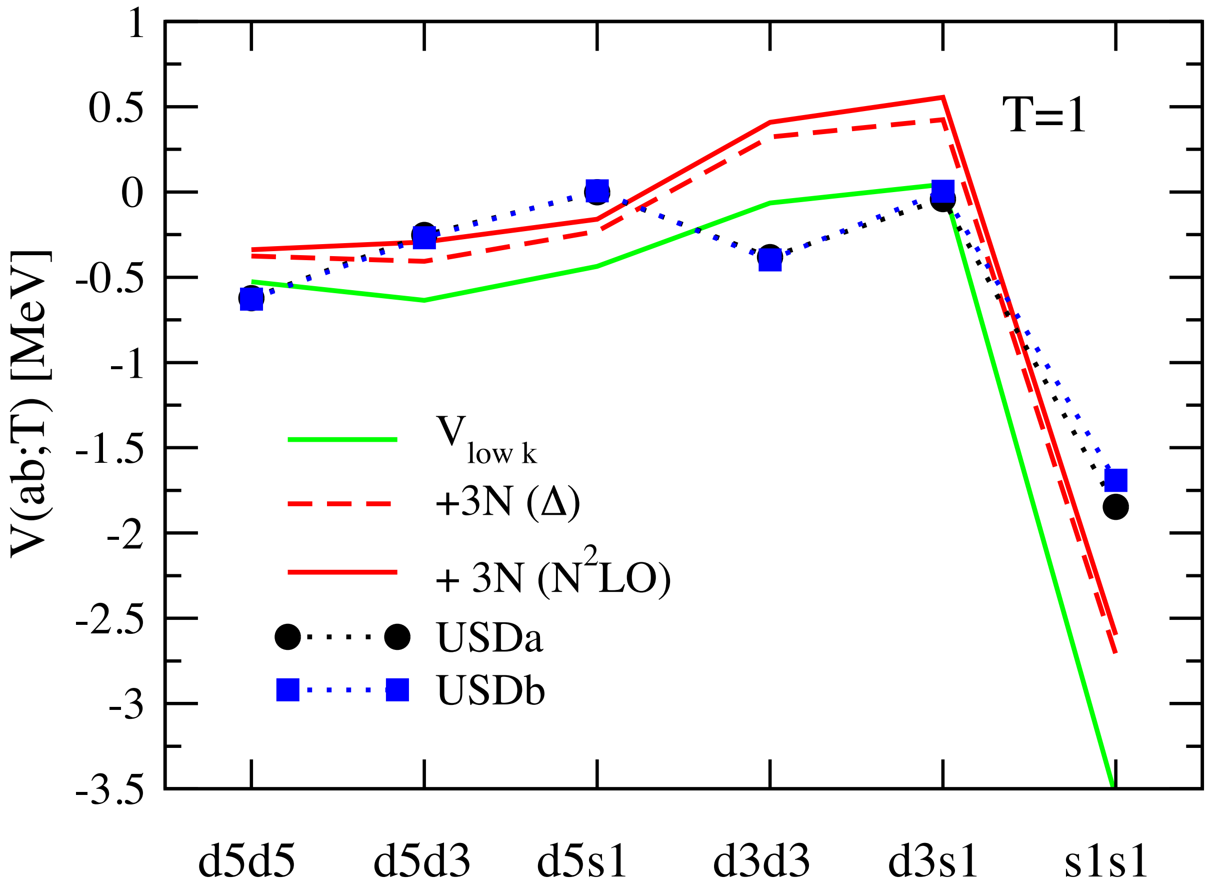
No gap at ^{22}O, yet enhanced closed-shell features (high 2^+, etc.)

Lee-Suzuki transformation into sd-shell

Usual shell gap emerges at ^{22}O

Similar evolution to USDb Hamiltonian

Two-body 3N: Monopoles in *sd*-shell



Dominant effect from
one-Δ – as expected
from cutoff variation

3N forces produce clear
repulsive shift in monopoles

First calculations to show missing monopole strength due to neglected 3N

Future: Improved treatment of high-lying orbits

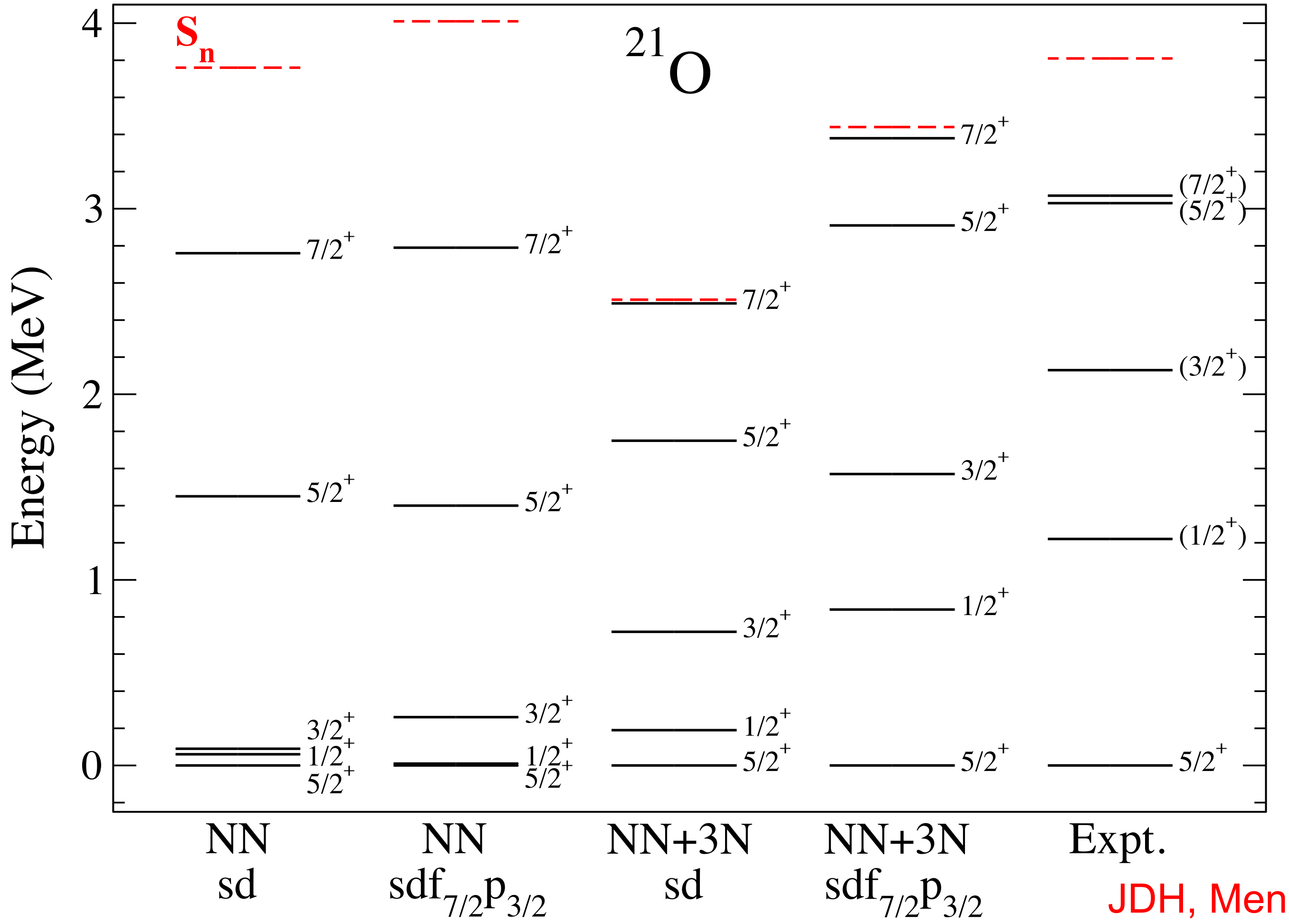
Treat as holes in ^{40}Ca core

Continuum effects

Impact on Spectra: ^{21}O

Neutron-rich oxygen spectra with NN+3N

Spectrum sensitive to $s_{1/2}$ shell closure



JDH, Menendez, Schwenk, EPJ (2013)

NN-only

Low-lying states

too compressed

$7/2^+$-$5/2^+$ too wide

Microscopic NN+3N

Improvement in *sd*

Extended orbits essential

Improved spacing in all levels

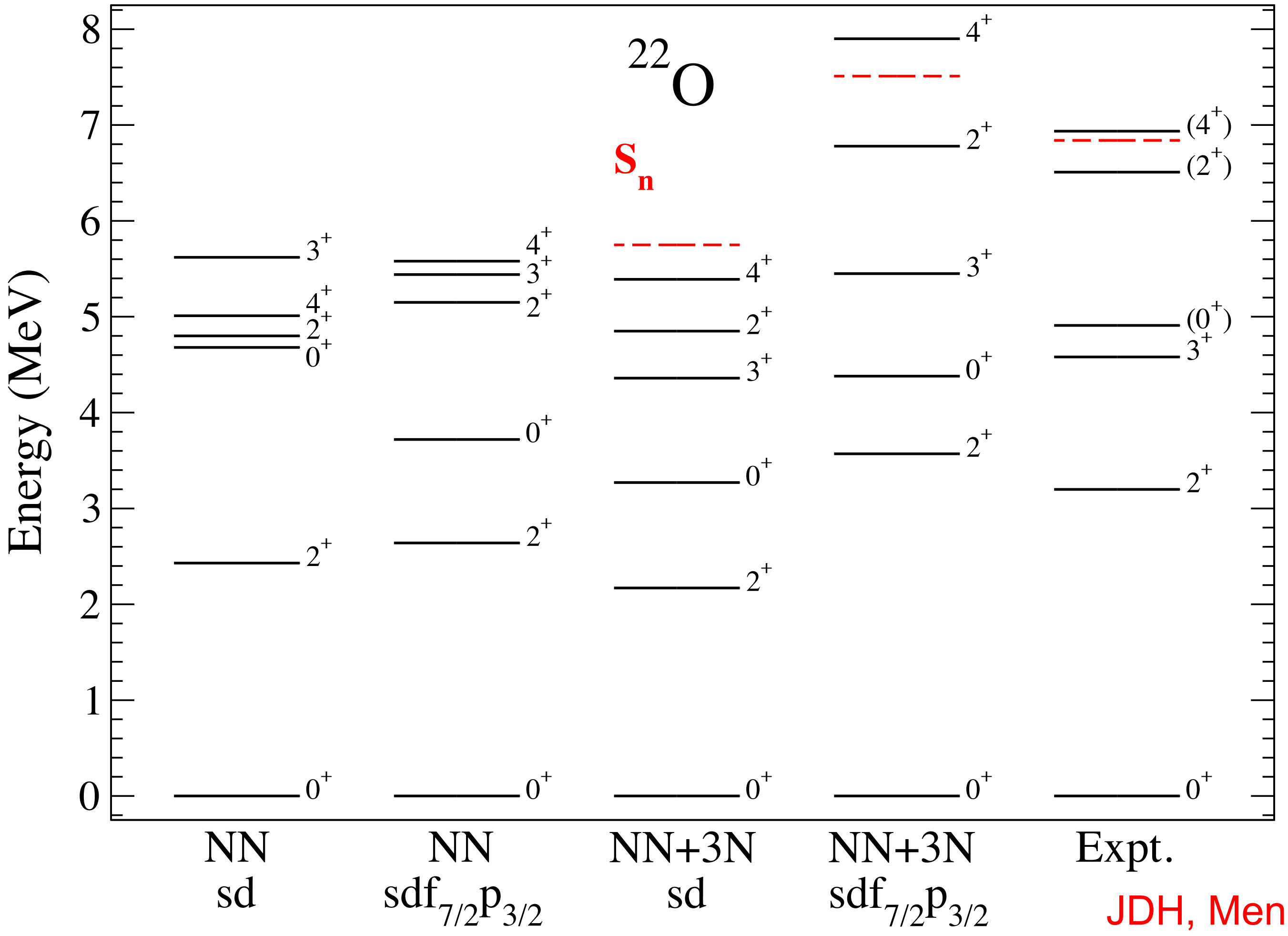
3N improvements largely due to higher calculated $s_{1/2}$ orbital

Need proper treatment of non-degenerate spaces

Impact on Spectra: ^{22}O

Neutron-rich oxygen spectra with NN+3N

^{22}O: $N=14$ new magic number – not reproduced with NN



NN-only

2^+ too low

Spectrum too compressed

Microscopic NN+3N

Extended space essential

Reproduces $N=14$ magic number

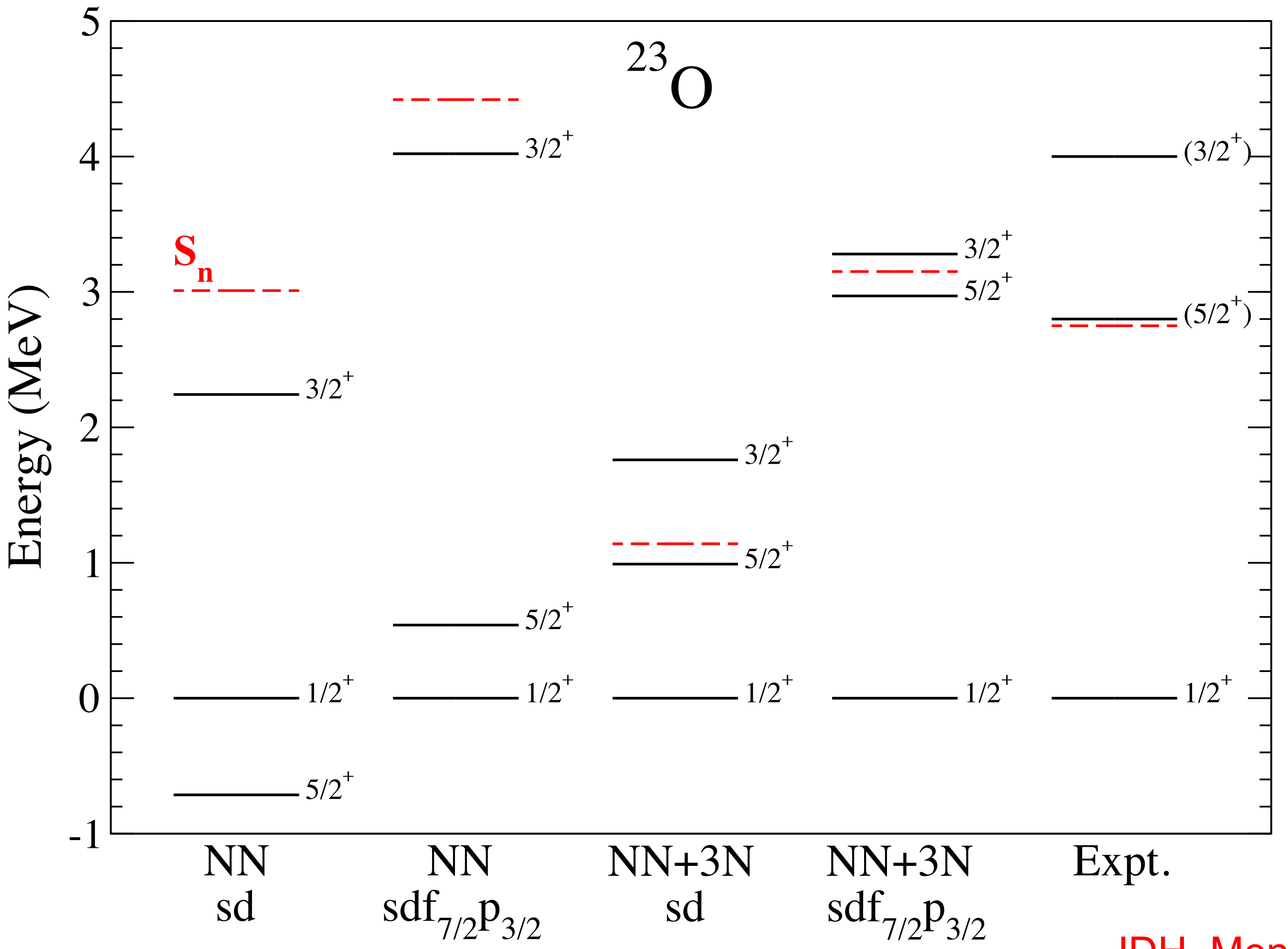
JDH, Menendez, Schwenk, EPJ (2013)

Contributions from 3N and extended valence orbitals important

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

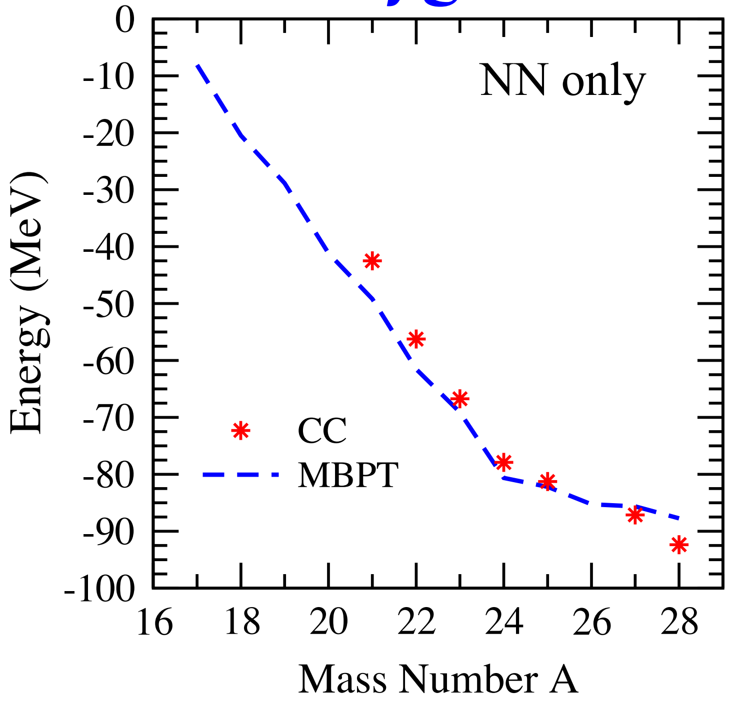
JDH, Menendez, Schwenk, EPJA (2013)

Coupled Cluster Benchmark

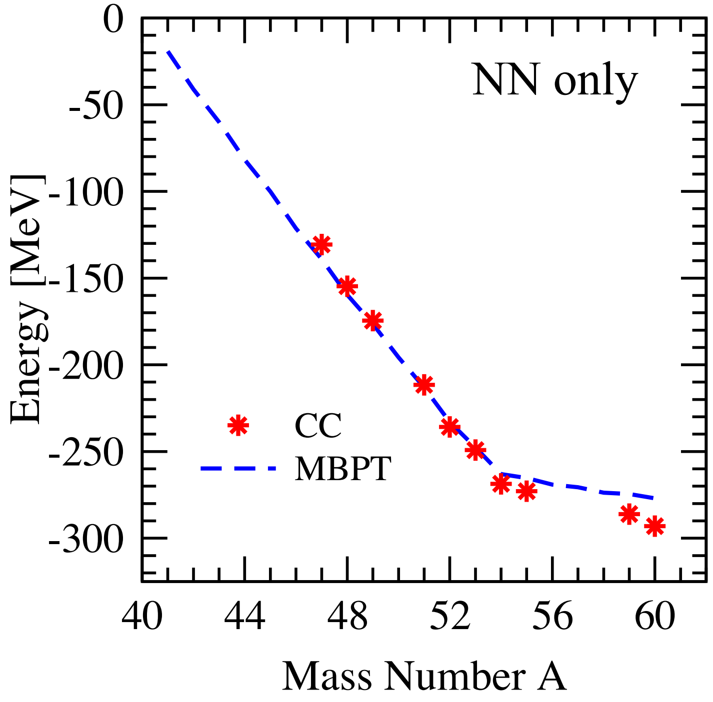
Benchmark against ab-initio Coupled-Cluster Theory

SPEs: one-particle attached CC energies in ^{17}O and ^{41}Ca

Oxygen



Calcium



Energies relative to ^{16}O and ^{40}Ca

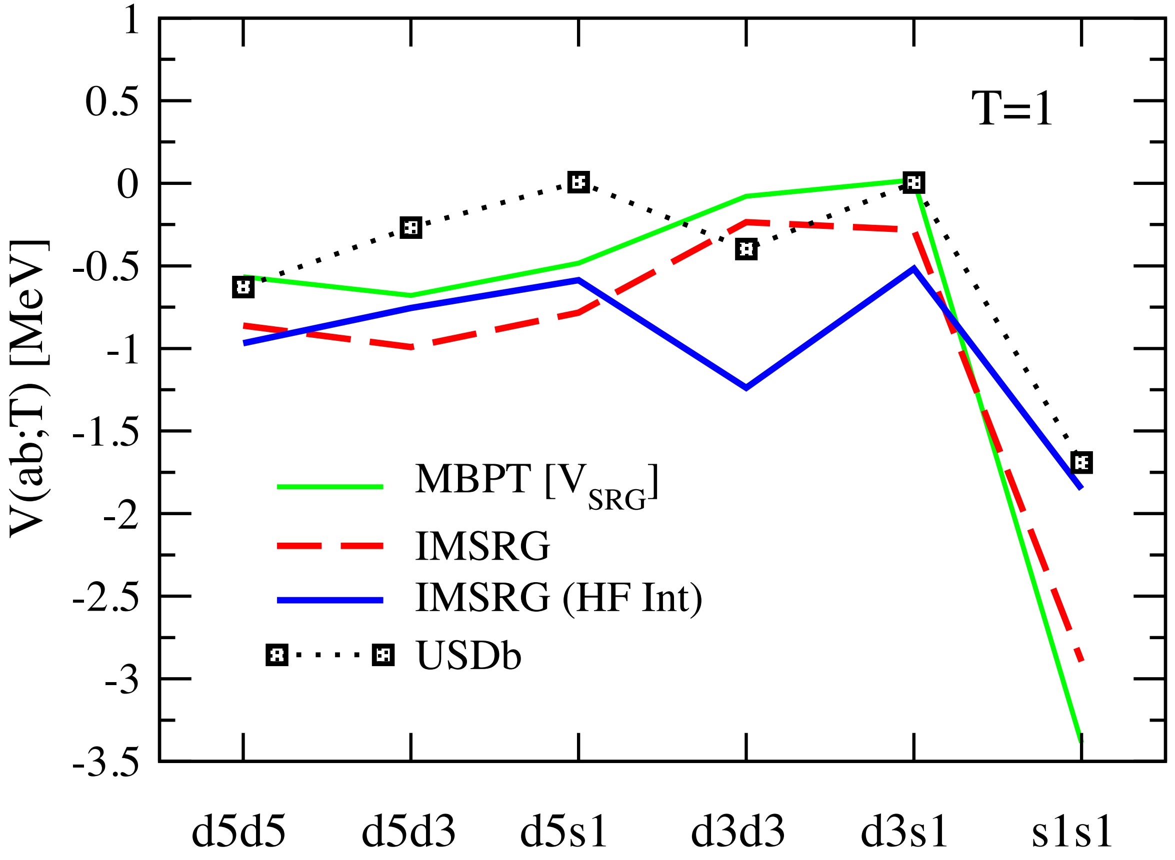
Small difference in many-body methods ~5%

Explore further benchmarks: NCSM, IM-SRG…

IM-SRG vs. MBPT: Monopoles

Monopoles: angular average of interaction

Determines interaction of orbit a with b; evolution of orbital energies



$$V_{ab}^{T} = \frac{\sum_J (2J+1)\ V_{abab}^{JT}}{\sum_J (2J+1)}$$

Similar trends in MBPT/IM-SRG – attractive shift in IM-SRG

Promising trends for IM-SRG in HF basis using intrinsic Hamiltonian

Perturbative vs. Nonperturbative SPEs

3N forces: additional repulsion improves SPEs

Orbit	USDb	MBPT NN	MBPT NN+3N	IM-SRG NN	IM-SRG NN+3N-ind	IM-SRG NN+3N-full
$d_{5/2}$	-3.93	-5.43	**-3.78**	-7.90	**-3.77**	**-4.62**
$s_{1/2}$	-3.21	-5.32	**-2.42**	-6.87	**-2.46**	**-2.96**
$d_{3/2}$	2.11	-0.97	**1.45**	1.41	**2.33**	**3.17**

JDH, Menendez, Schwenk, EPJA (2013)
Bogner et al., PRL (2014)

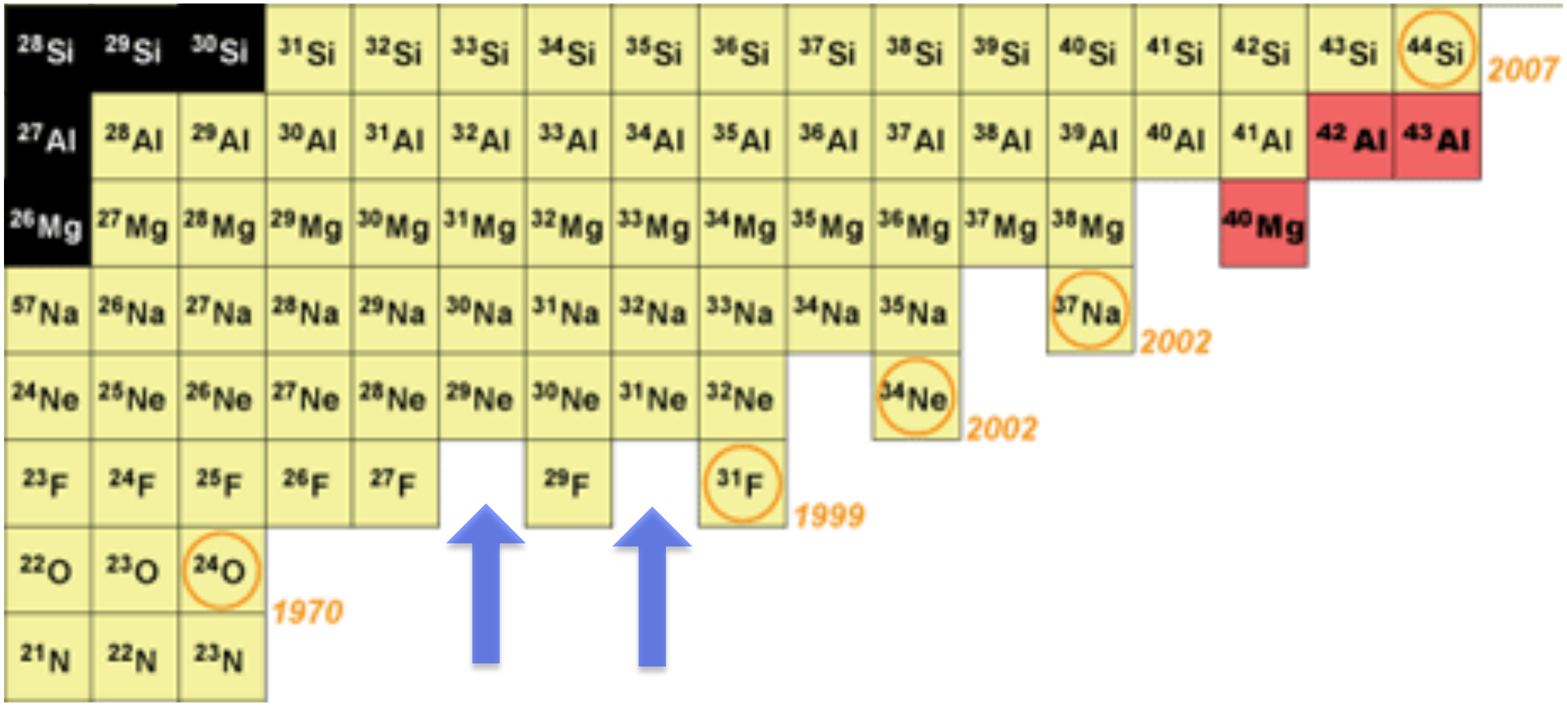
Similar contributions in standard/extended valence spaces

Comparable with phenomenology

Towards Full sd-Shell: Fluorine

Next challenge: **valence protons + neutrons**

Explore physics of neutron-rich fluorine and neon isotopes



Prediction of unbound ^{28,30}F

Agrees well with phenomenology

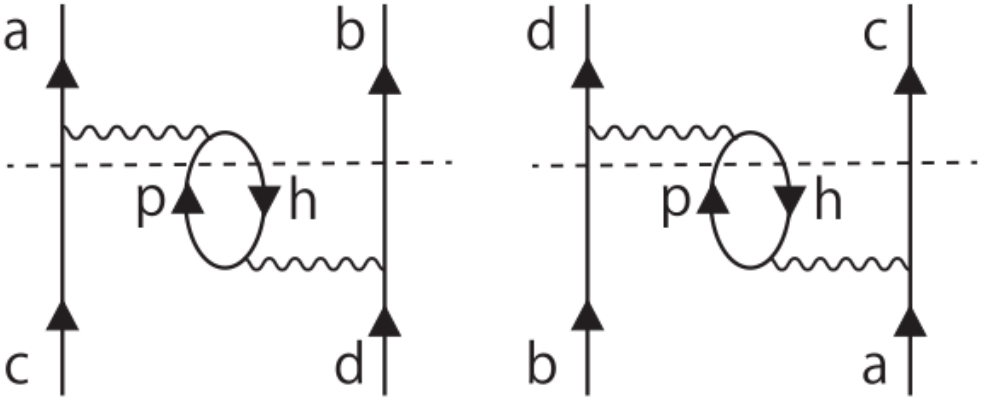
$S_n(^{28}F)$	SDPF-U	NN+3N	AME 2011
	-451 keV	-458 keV	-419 keV

JDH, Menendez, Schwenk, in prep.

Non-Degenerate Valence Space Theory

Strong non-Hermiticity (or divergence) for non-degenerate valence space:

$$\frac{1}{\varepsilon_d - \varepsilon_b - \varepsilon_p - \varepsilon_h}$$



$$\frac{1}{\varepsilon_a - \varepsilon_c - \varepsilon_p - \varepsilon_h}$$

Idea: replace starting energy with arbitrary parameter $\omega = PH_0P \rightarrow E$

In both cases: $\frac{1}{E - (\varepsilon_c + \varepsilon_p + \varepsilon_b - \varepsilon_h)}$ avoids divergence and non-Hermiticity

Final results should not depend on E – true when folded diagrams are calculated

Required for use of Hartree-Fock basis

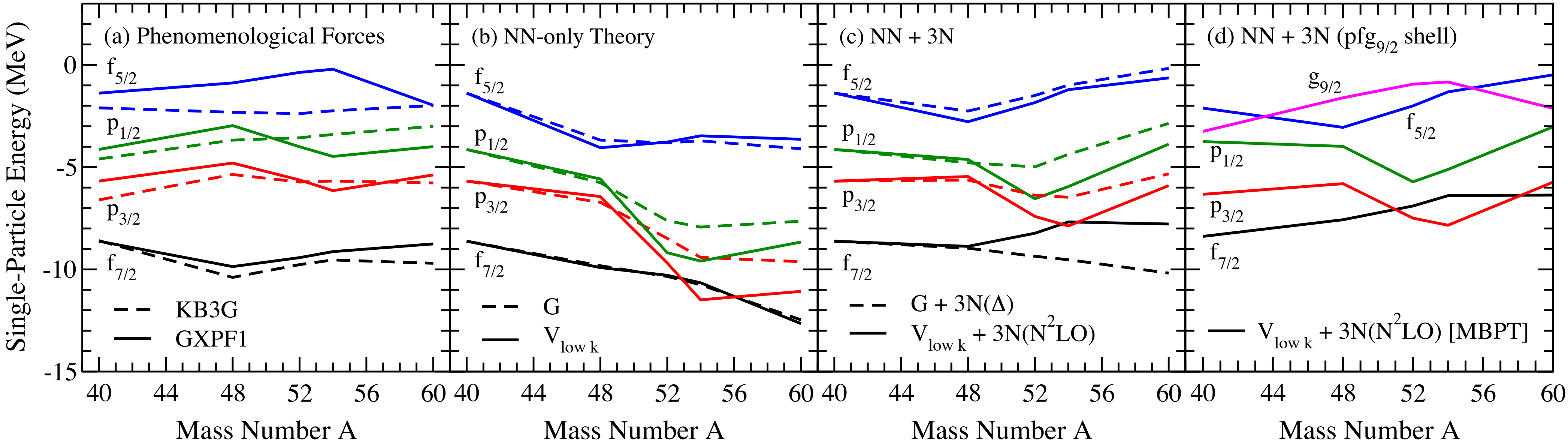
Test calculations show **more attractive cross-shell monopoles**

Lower $f_{7/2}$ $p_{3/2}$ orbitals for neutron-rich F, Ne

Backup Calcium

Evolution of Shell Structure

SPE evolution with 3N forces in *pf* and $pfg_{9/2}$ spaces:



NN+3N *pf*-shell:

JDH, Otsuka, Schwenk, Suzuki JPG (2012)

Trend across: improved binding energies

Increased gap at ^{48}Ca: enhanced closed-shell features

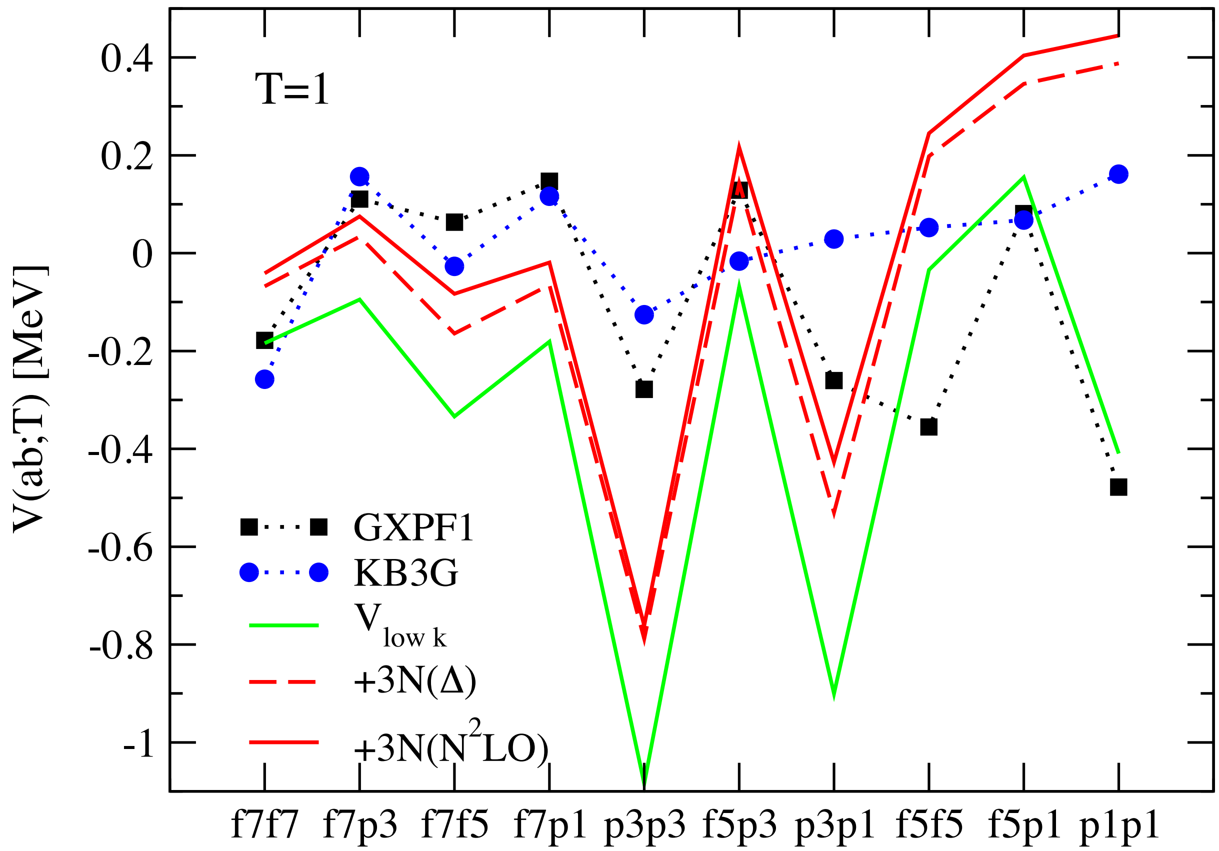
Include $g_{9/2}$ orbit, calculated SPEs

Different behavior of ESPEs (not observable, model dependent)

Small gap can give large 2^+ energy: due to many-body correlations

Duguet, Hagen, PRC (2012)
Duguet, Hergert, JDH, Soma, in prep.

Two-body 3N: Monopoles in *pf*-shell



Dominant effect from **one-Δ** – as expected from cutoff variation

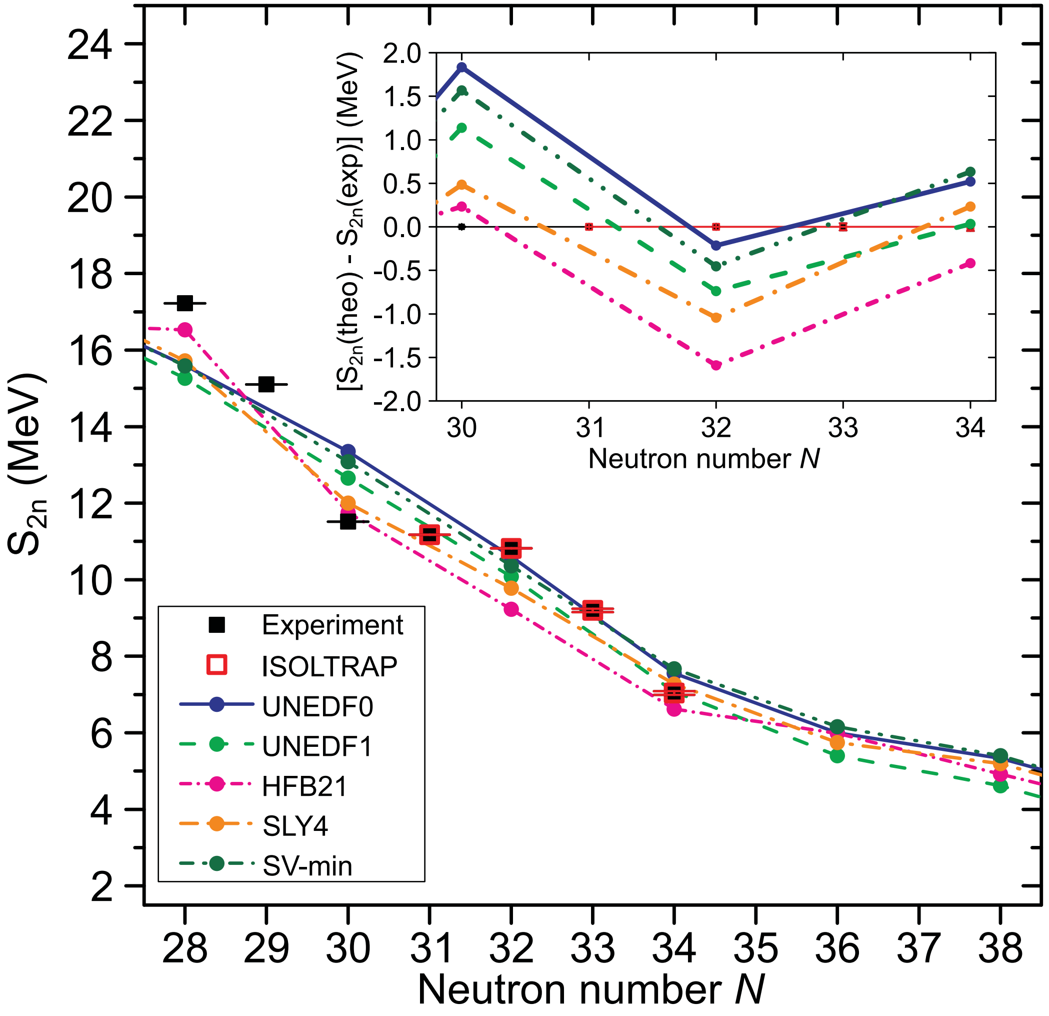
3N forces produce clear repulsive shift in monopoles

Similar to *sd*-shell

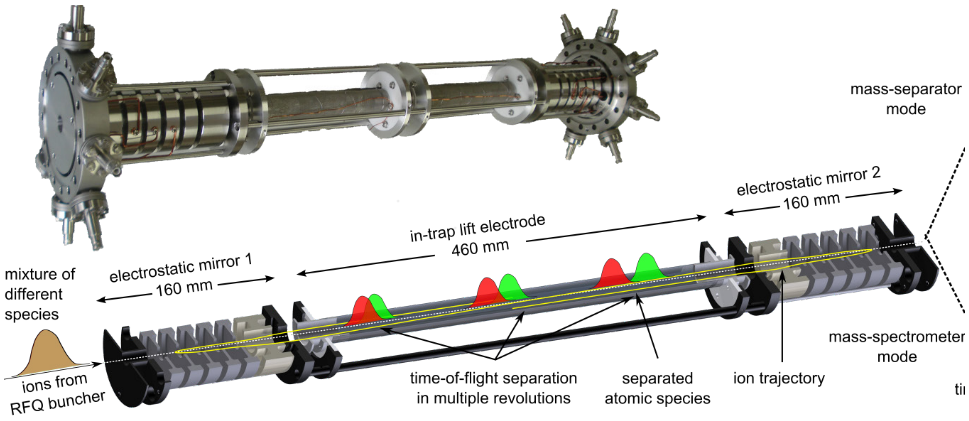
First calculations to show missing monopole strength due to neglected 3N

Experimental Connection: Mass of ^{54}Ca

New precision mass measurement of ^{53,54}Ca at **ISOLTRAP**: multi-reflection ToF



Wienholtz et al., Nature (2013)



ISOLTRAP ***Measurement***

Sharp decrease past ^{52}Ca

Unambiguous closed-shell ^{52}Ca

Test predictions of various models

EDF Calculations

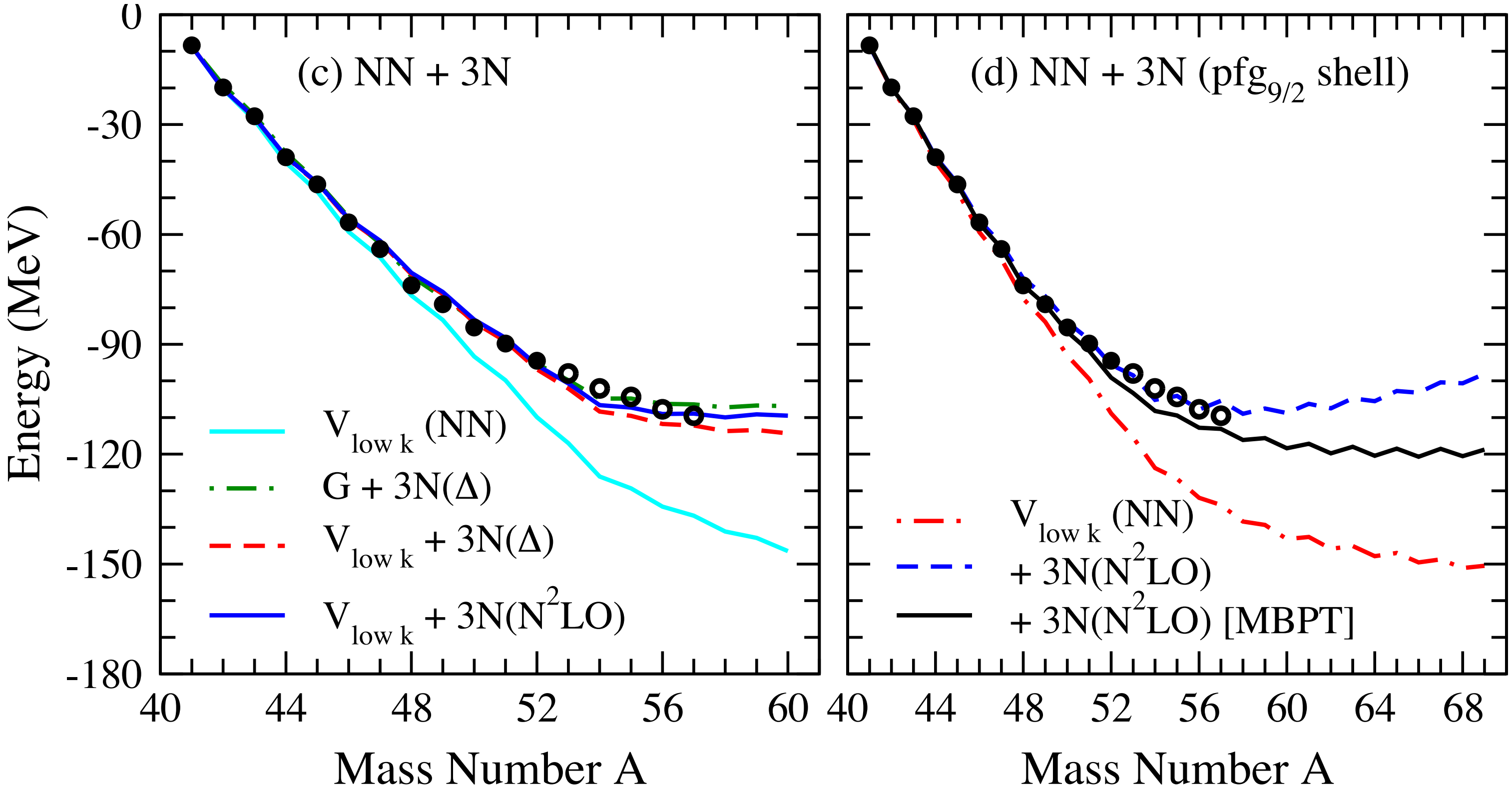
Reasonable overall trend

Closed-shell features not reproduced for ^{48,52}Ca

Calcium Ground State Energies and Dripline

Ground state energies using NN+3N

NN-only: overbinds beyond ~ ^{46}Ca



Holt, Otsuka, Schwenk, Suzuki, JPG (2012)

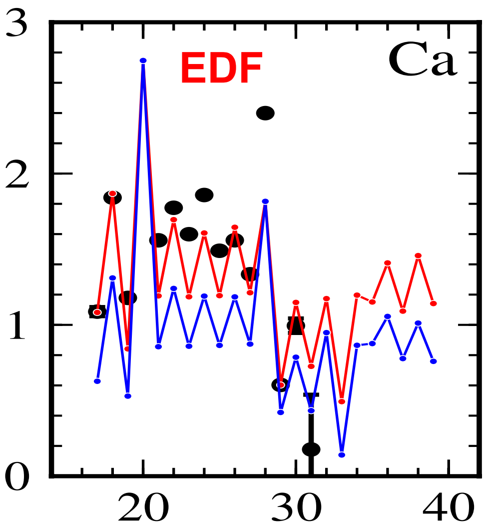
***pf*-shell**: 3N forces correct binding energies; good experimental agreement

***pfg*$_{9/2}$-shell**: calculate to ^{70}Ca; modest overbinding near ^{52}Ca

Heaviest calcium isotope ~ $^{58\text{-}60}$Ca; flat behavior past ^{54}Ca

Pairing in Calcium Isotopes: Ladders

Compare with $\Delta_n^{(3)}$ calculated from microscopic NN+3N in calcium



HFB iterates ladders microscopically in pairing channel

Compare with ***pp, hh* ladders to 3rd order**

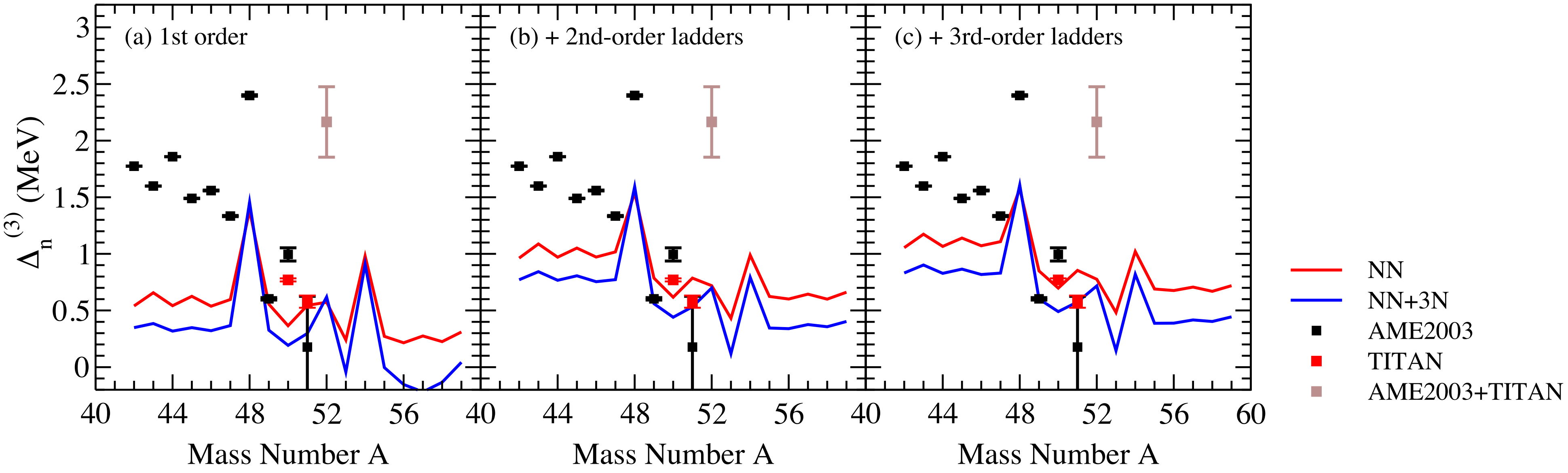
Improved agreement with experiment

Convergence in order-by-order ladders

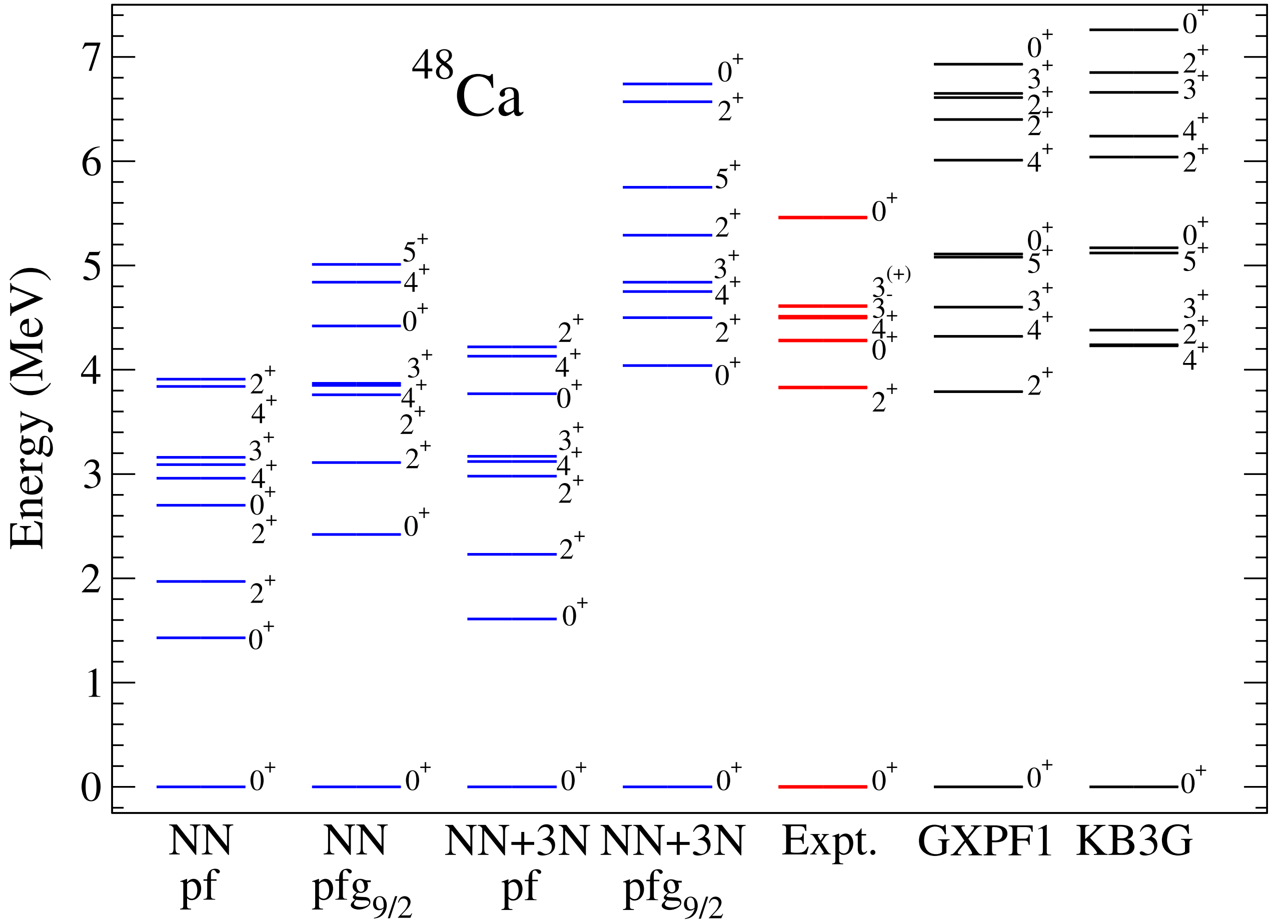
Suppression from 3N forces as in EDF

Incorrect odd/even staggering

JDH, Menendez, Schwenk, in prep



N=28 Magic Number in Calcium: Spectrum



JDH, Menendez, Schwenk, in prep.

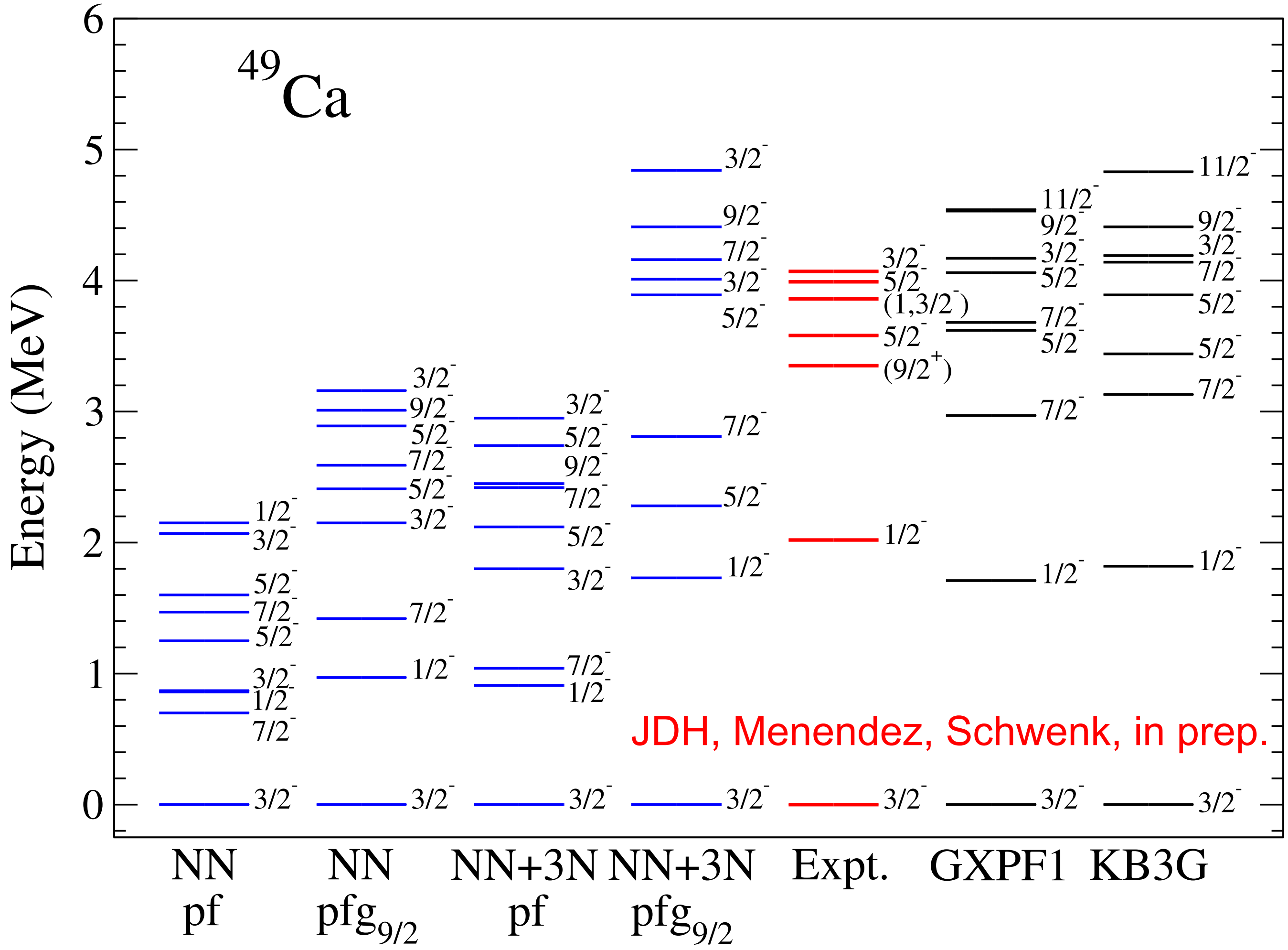
Generally spectrum too compressed

***$pfg_{9/2}$*-shell**: With NN+3N spectrum comparable to phenomenology

Both 3N and extended space essential

Impact on Spectra: ^{49}Ca

Neutron-rich calcium spectra with NN+3N



JDH, Menendez, Schwenk, in prep.

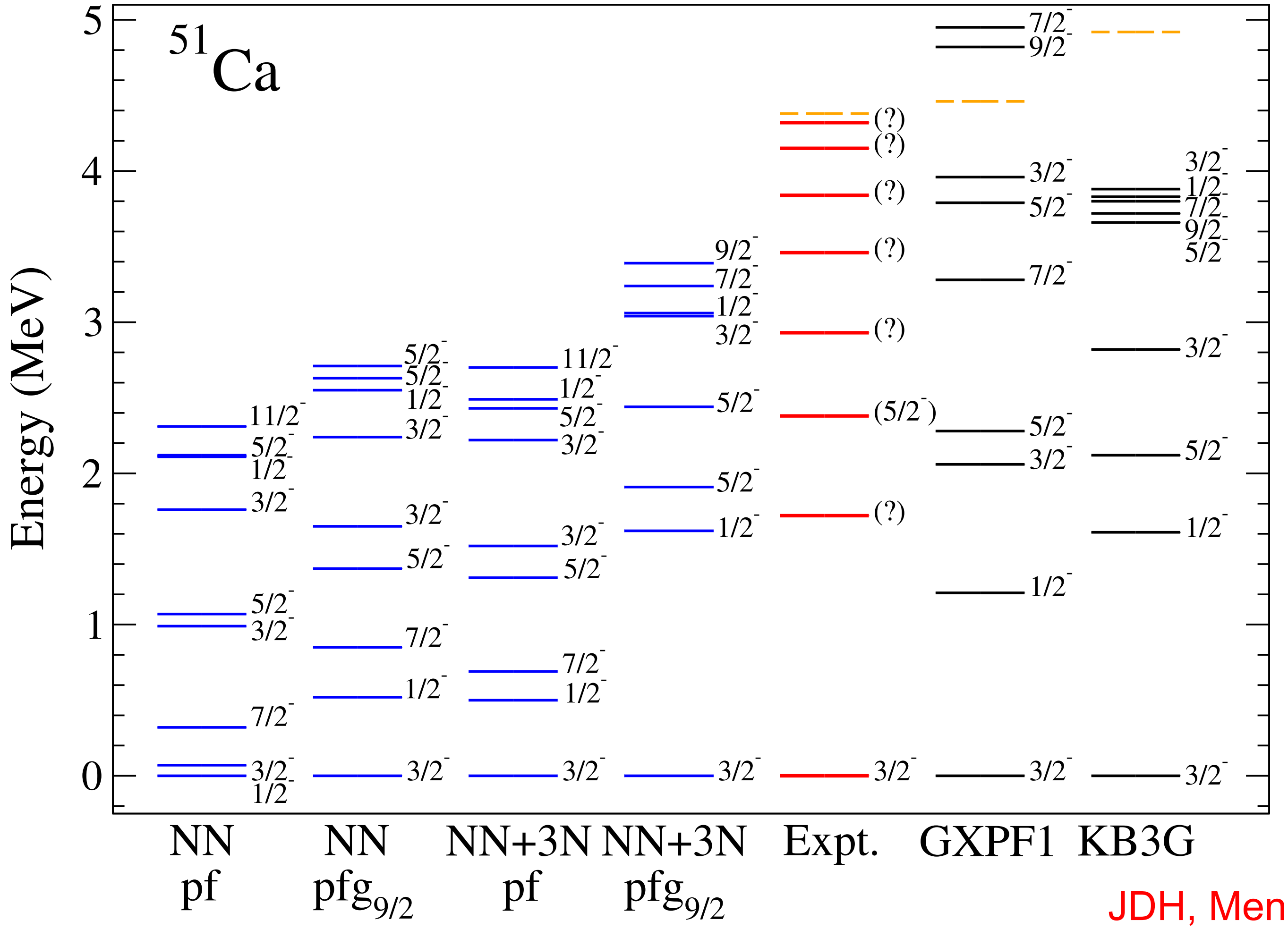
Spectrum typically too compressed

NN+3N in $pfg_{9/2}$ correct $1/2^-$

Comparable to phenomenology (as for all lighter Ca isotopes)

Impact on Spectra: ^{51}Ca

Neutron-rich calcium spectra with NN+3N



JDH, Menendez, Simonis, Schwenk, in prep.

Possibility to assign spin/parity where unknown

Gamma-ray spectroscopy needed

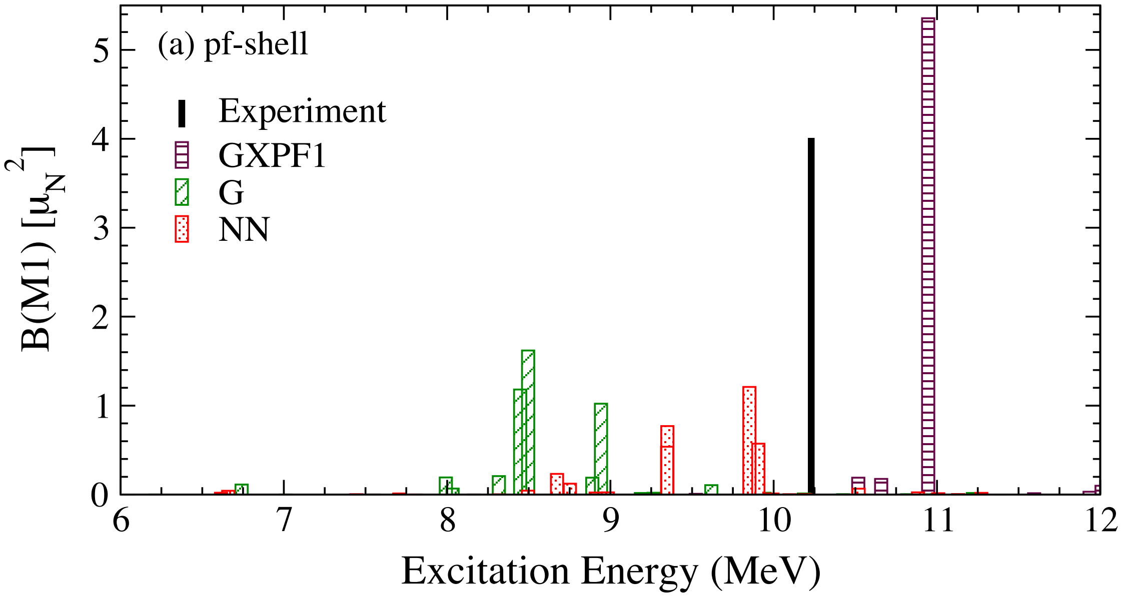
N=28 Magic Number: *M1* Transition Strength

$B(M1:0^+_{gs} \rightarrow 1^+)$ concentration indicates a single particle (spin-flip) transition

von Neumann-Coesel, *et al*. (1998)

Not reproduced in phenomenology

NN-only: highly fragmented strength, well below experiment



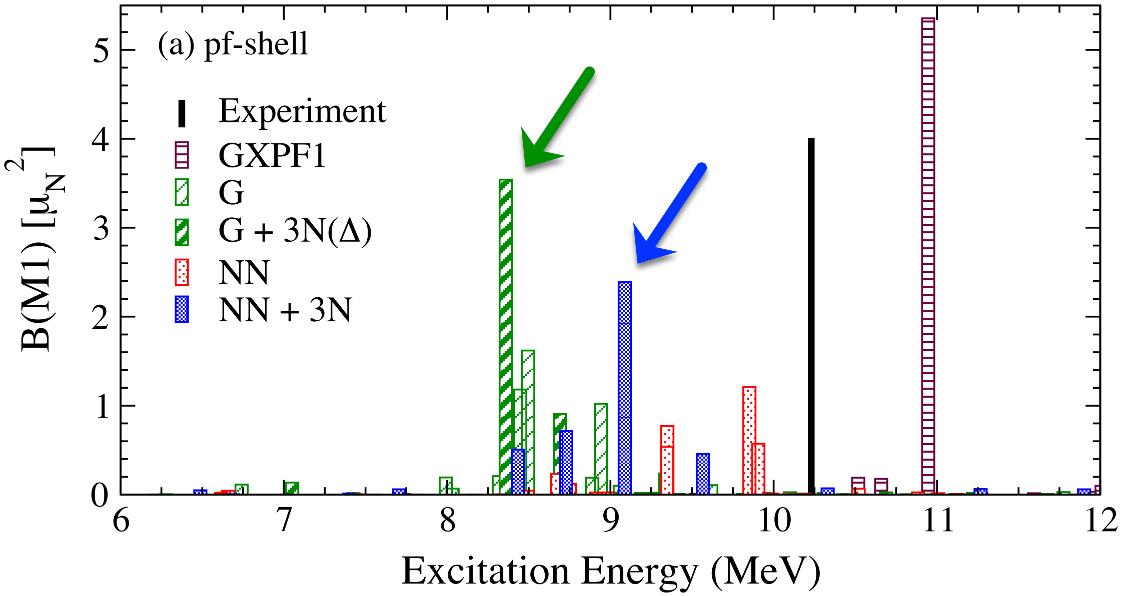
N=28 Magic Number: *M1* Transition Strength

$B(M1:0^+_{gs} \rightarrow 1^+)$ concentration indicates a single particle (spin-flip) transition

Not reproduced in phenomenology

von Neumann-Coesel, *et al*. (1998)

NN-only: highly fragmented strength, well below experiment



***pf*-shell**:

3N concentrates strength

Peaks below experiment

JDH, Otsuka, Schwenk, Suzuki, JPG (2012)

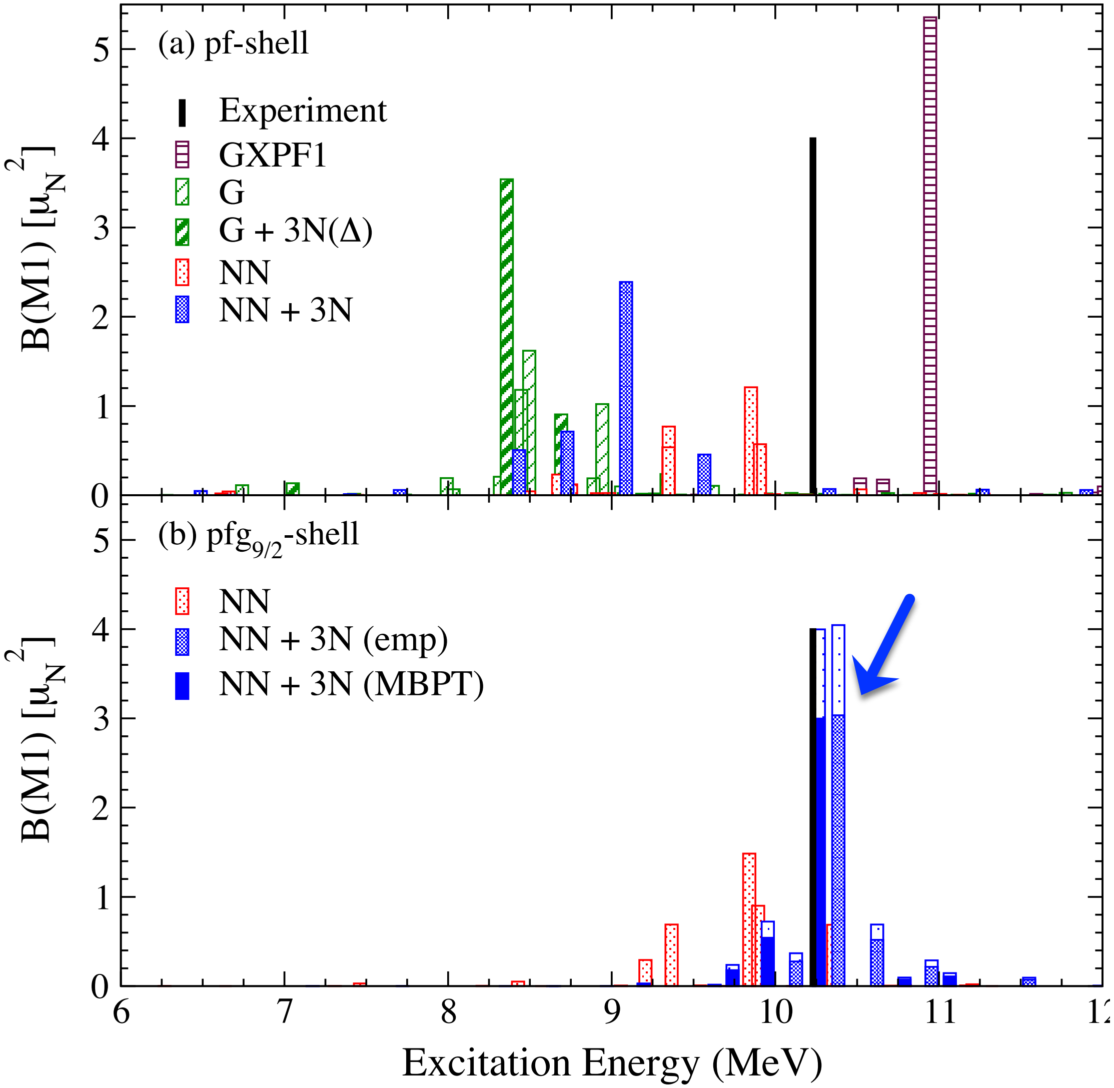
N=28 Magic Number: *M1* Transition Strength

$B(M1:0^+_{gs} \rightarrow 1^+)$ concentration indicates a single particle (spin-flip) transition

von Neumann-Coesel, *et al*. (1998)

Not reproduced in phenomenology

NN-only: highly fragmented strength, well below experiment



***pf*-shell**:

3N concentrates strength

Peaks below experiment

JDH, Otsuka, Schwenk, Suzuki, JPG (2012)

***pfg*$_{9/2}$-shell**:

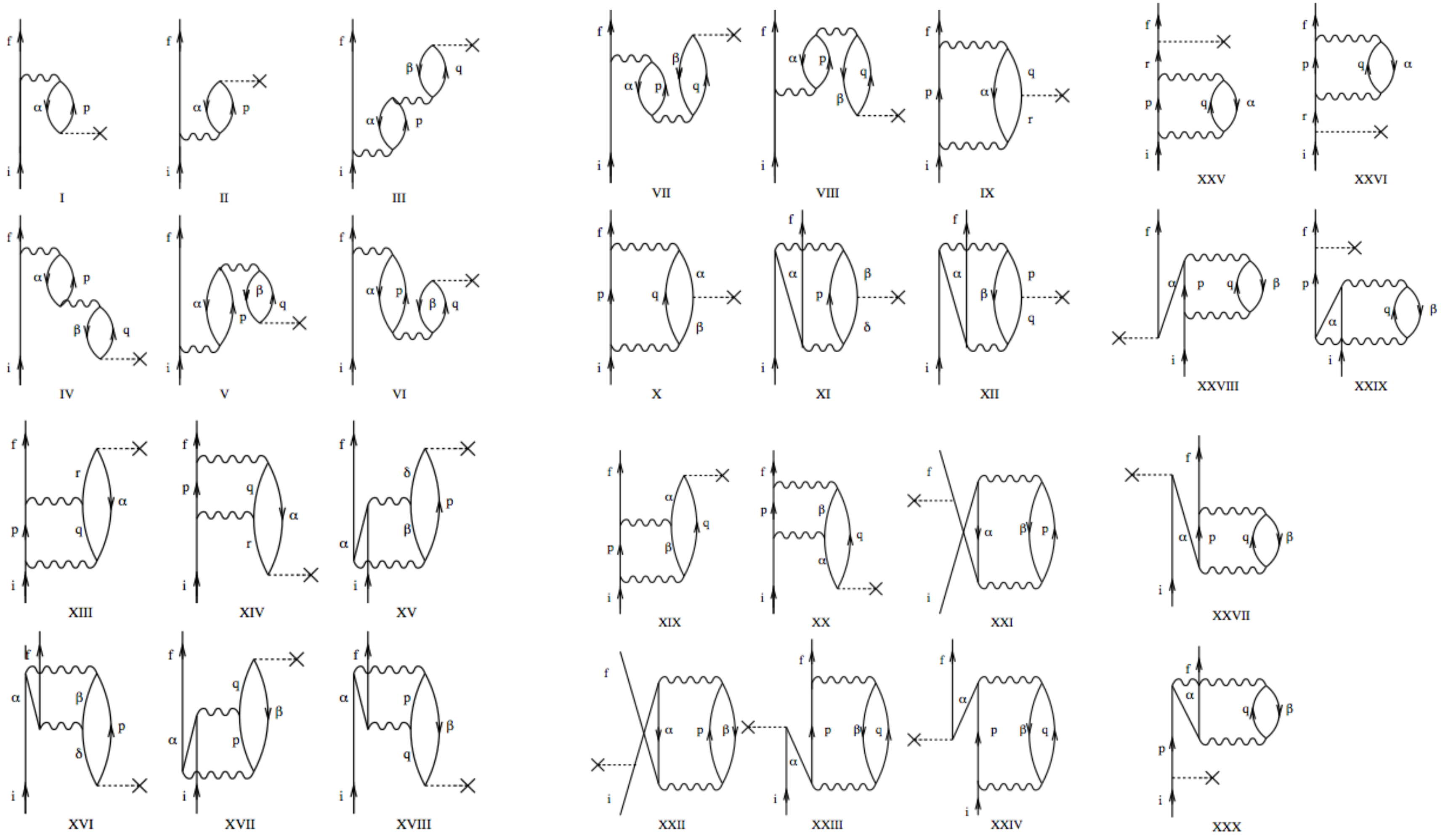
3N gives additional concentration

Peak close to experimental energy

Supports *N=28* magic number

Effective Operators

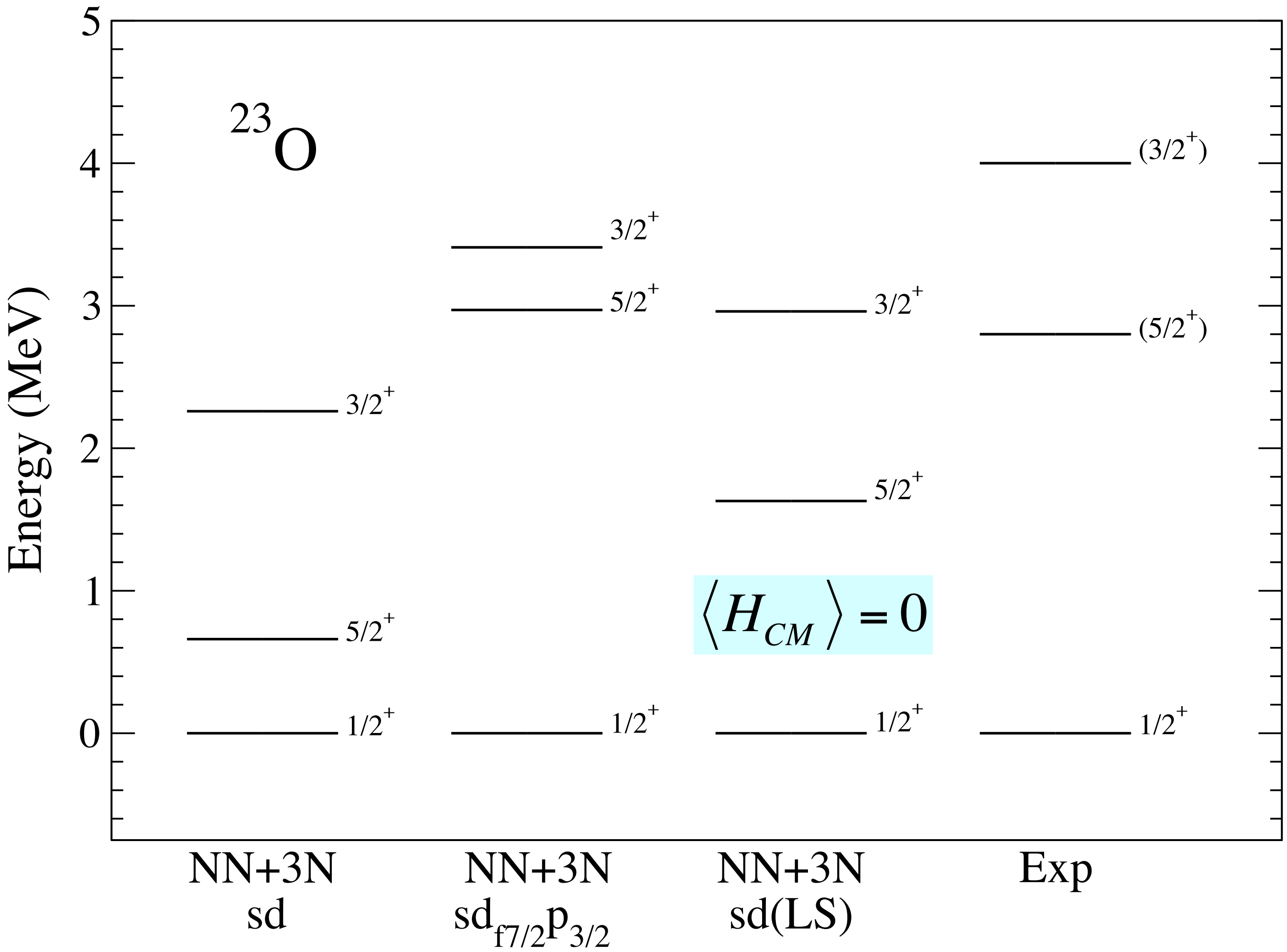
Investigate many-body effects on effective charges and quenching of g_A



Use low-momentum interactions and 3N forces

Evaluating Center-of-Mass Contamination

Apply new H_{eff}^{LS} to calculate spectra in neutron-rich oxygen

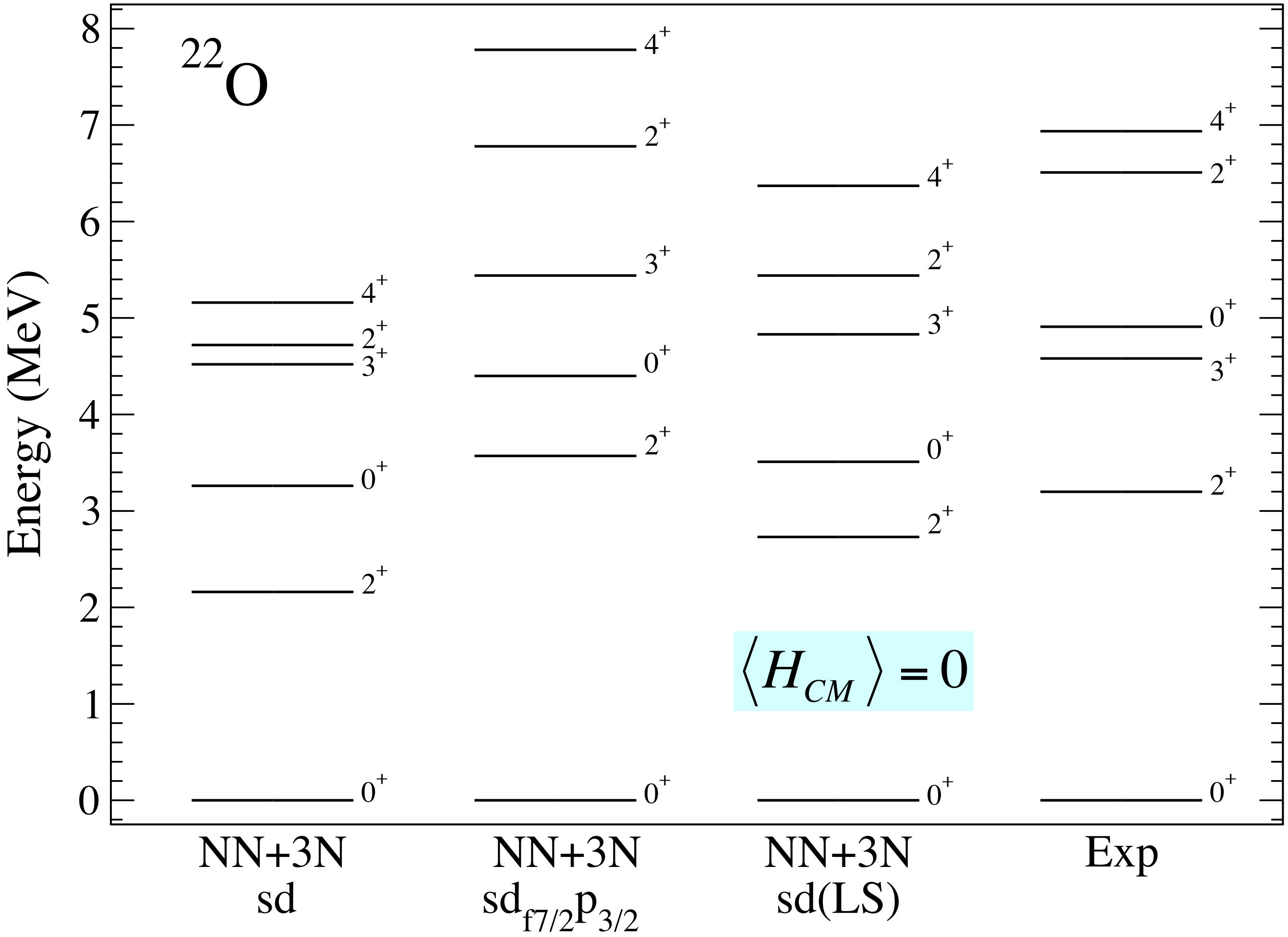


Clear improvement from standard *sd*-shell – not due to center of mass

Missing physics involving $N > 2$ neutrons in extended space

Evaluating Center-of-Mass Contamination

Apply new H_{eff}^{LS} to calculate spectra in neutron-rich oxygen

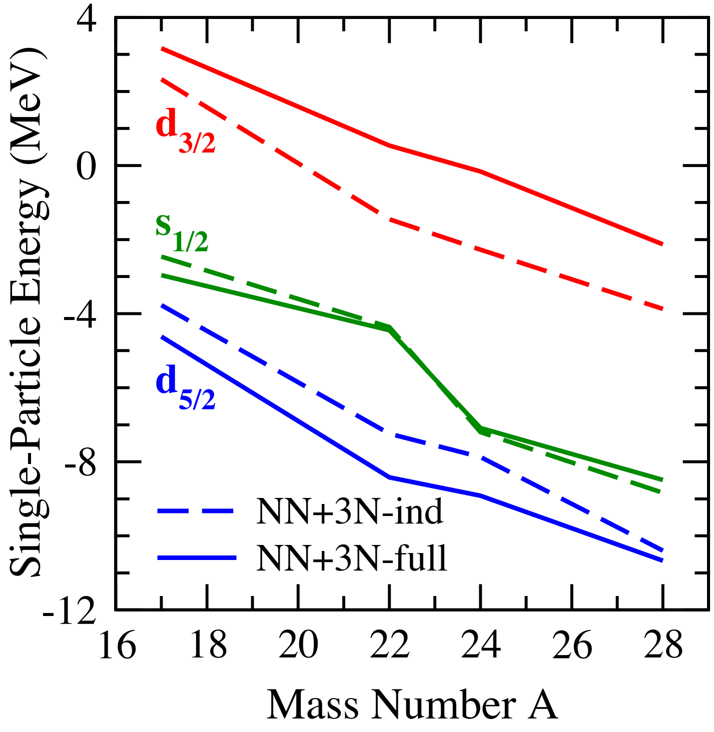


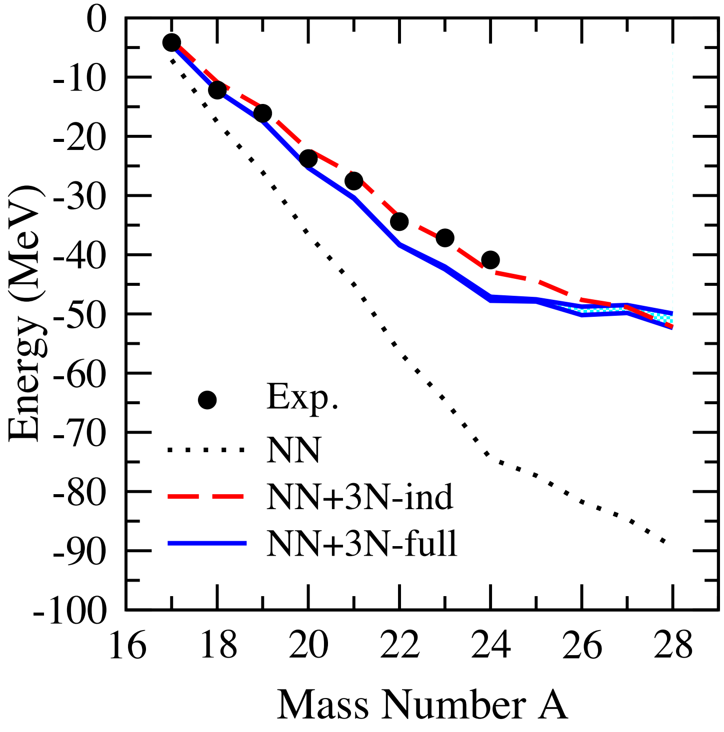
Improvements from standard *sd*-shell – not due to center of mass

Work in progress: involving $N > 2$ neutrons in extended space

IM-SRG Oxygen Ground-State Energies

Valence-space interaction and SPEs from NN+3N in *sd*-shell



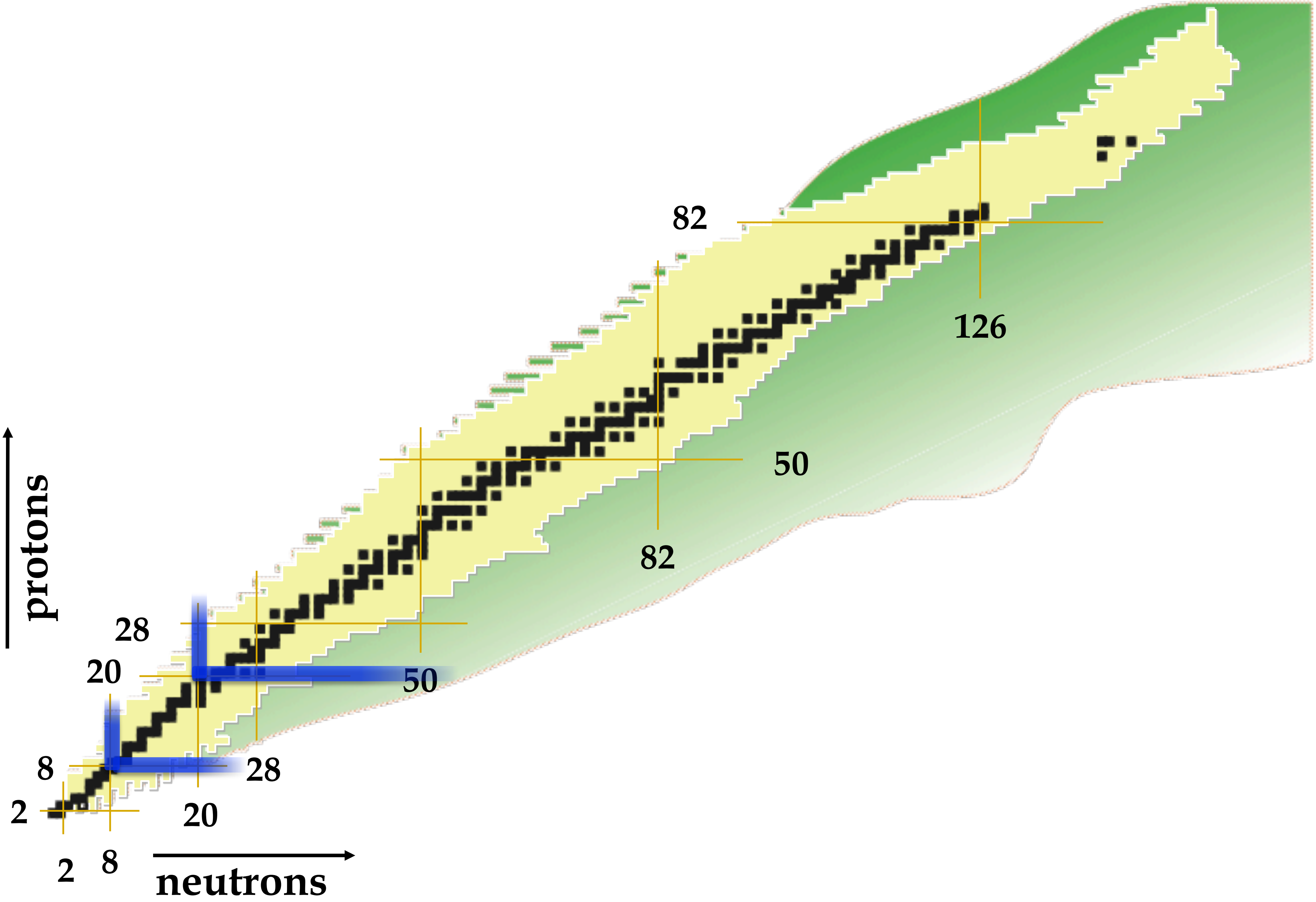


Hergert, JDH, Bogner, Schwenk, in prep.

Repulsive 3N gives unbound $d_{3/2}$

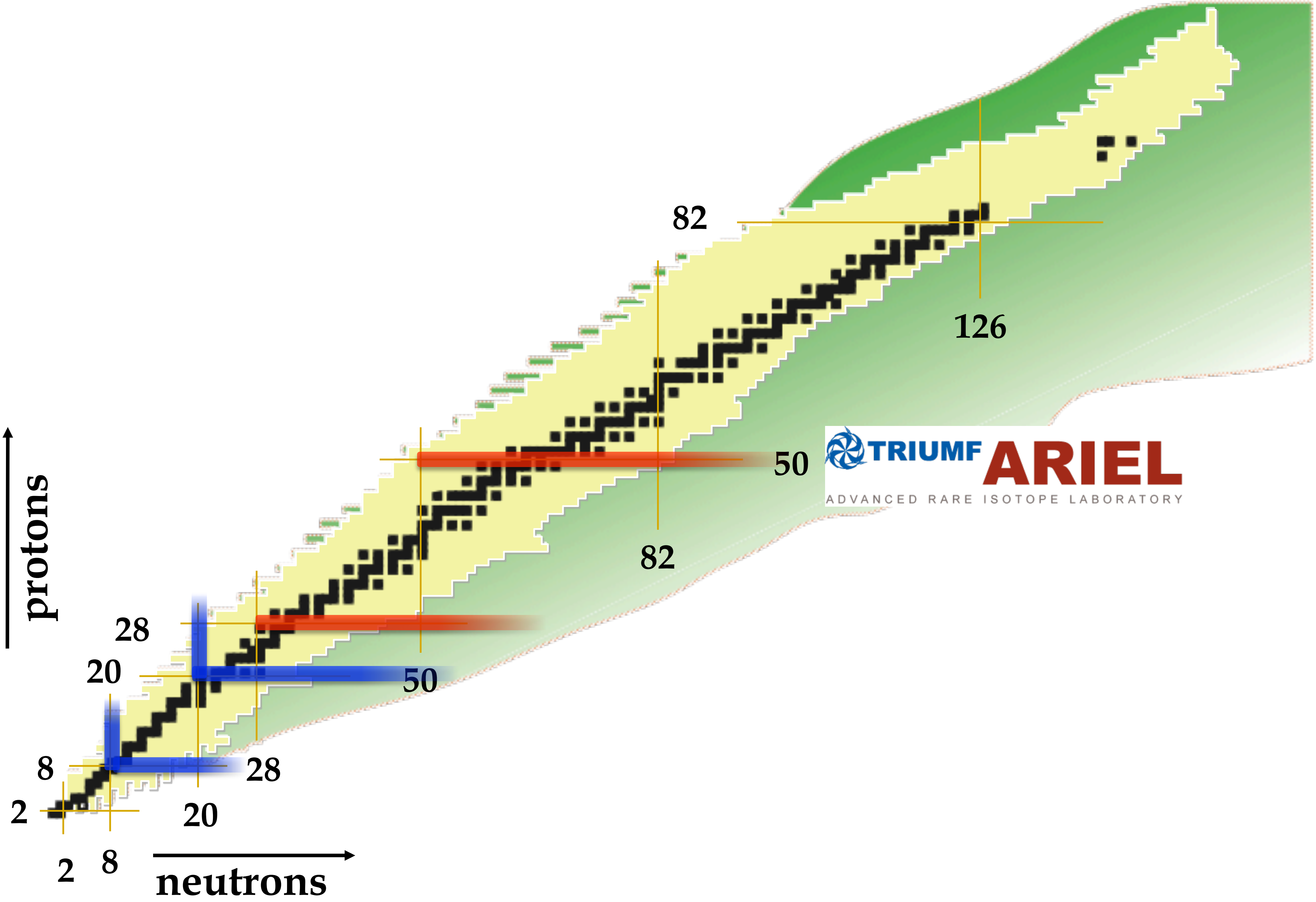
Good dripline properties

New Directions and Outlook



New Directions and Outlook

Heavier semi-magic chains: Nickel and Tin



New Directions and Outlook

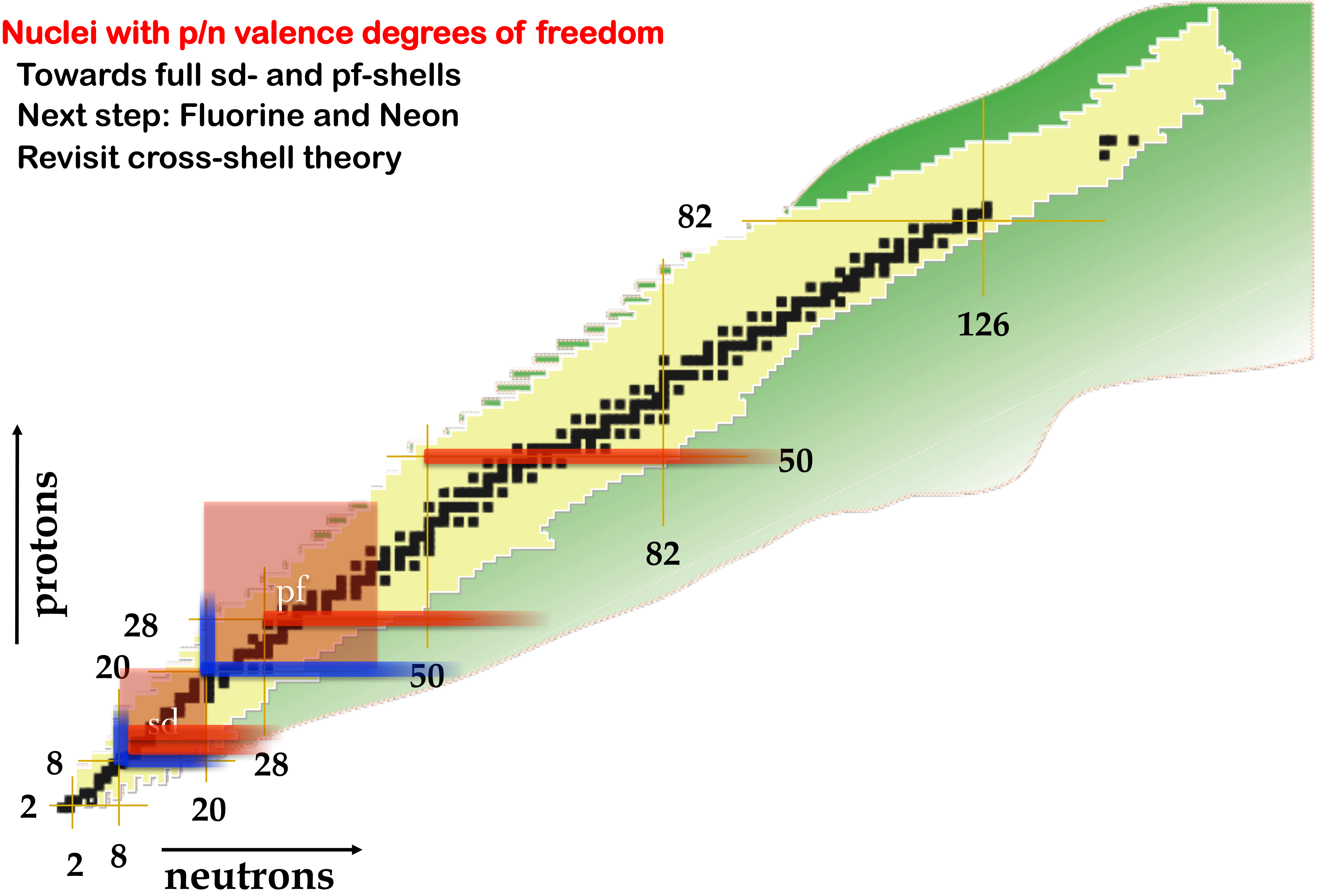
Heavier semi-magic chains: Nickel and Tin

Nuclei with p/n valence degrees of freedom

Towards full sd- and pf-shells

Next step: Fluorine and Neon

Revisit cross-shell theory



New Directions and Outlook

Heavier semi-magic chains: Nickel and Tin

Nuclei with p/n valence degrees of freedom

Towards full sd- and pf-shells

First step: Fluorine and Neon

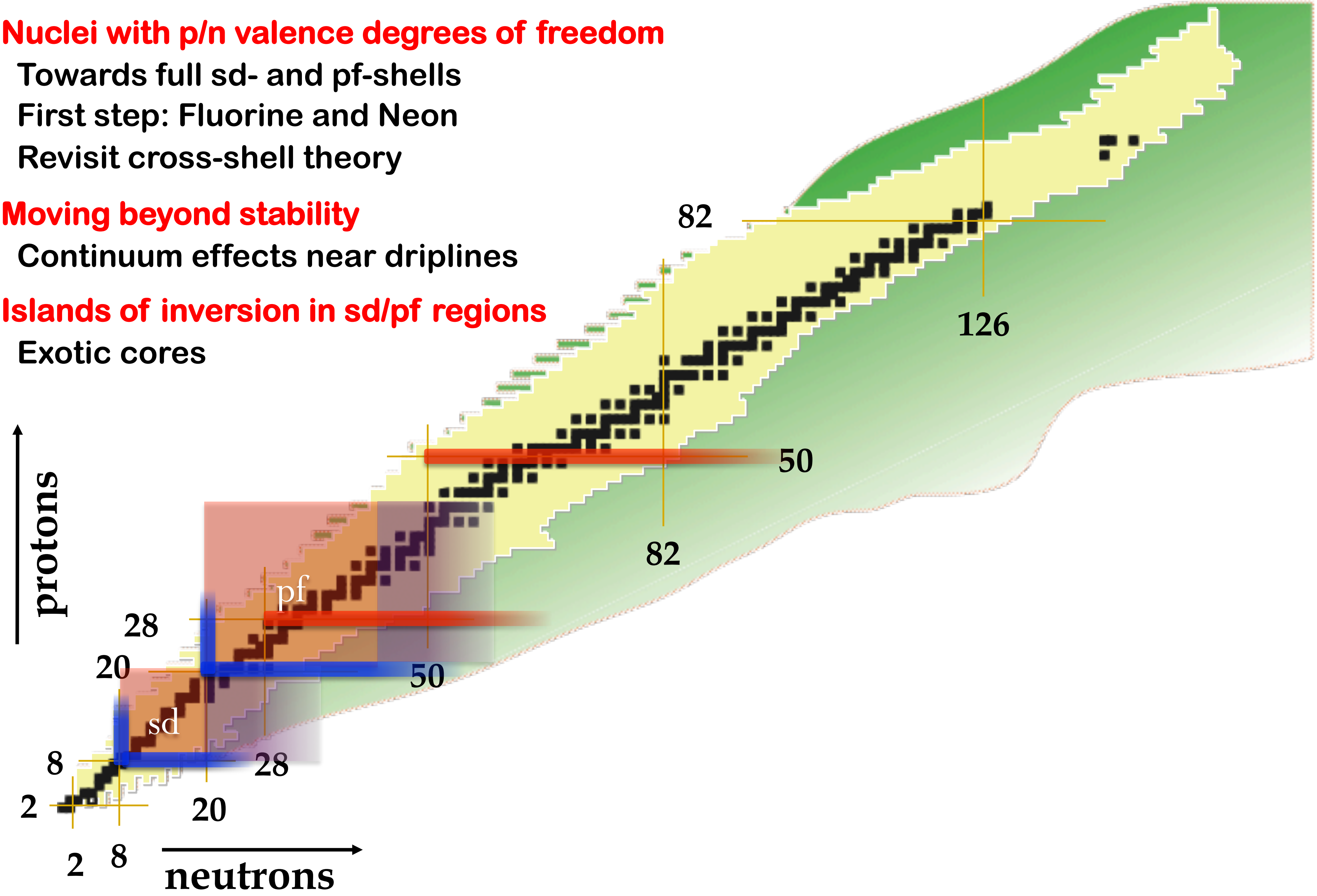
Revisit cross-shell theory

Moving beyond stability

Continuum effects near driplines

Islands of inversion in sd/pf regions

Exotic cores



New Directions and Outlook

Heavier semi-magic chains: Nickel and Tin

Nuclei with p/n valence degrees of freedom

Towards full sd- and pf-shells

First step: Fluorine and Neon

Revisit cross-shell theory

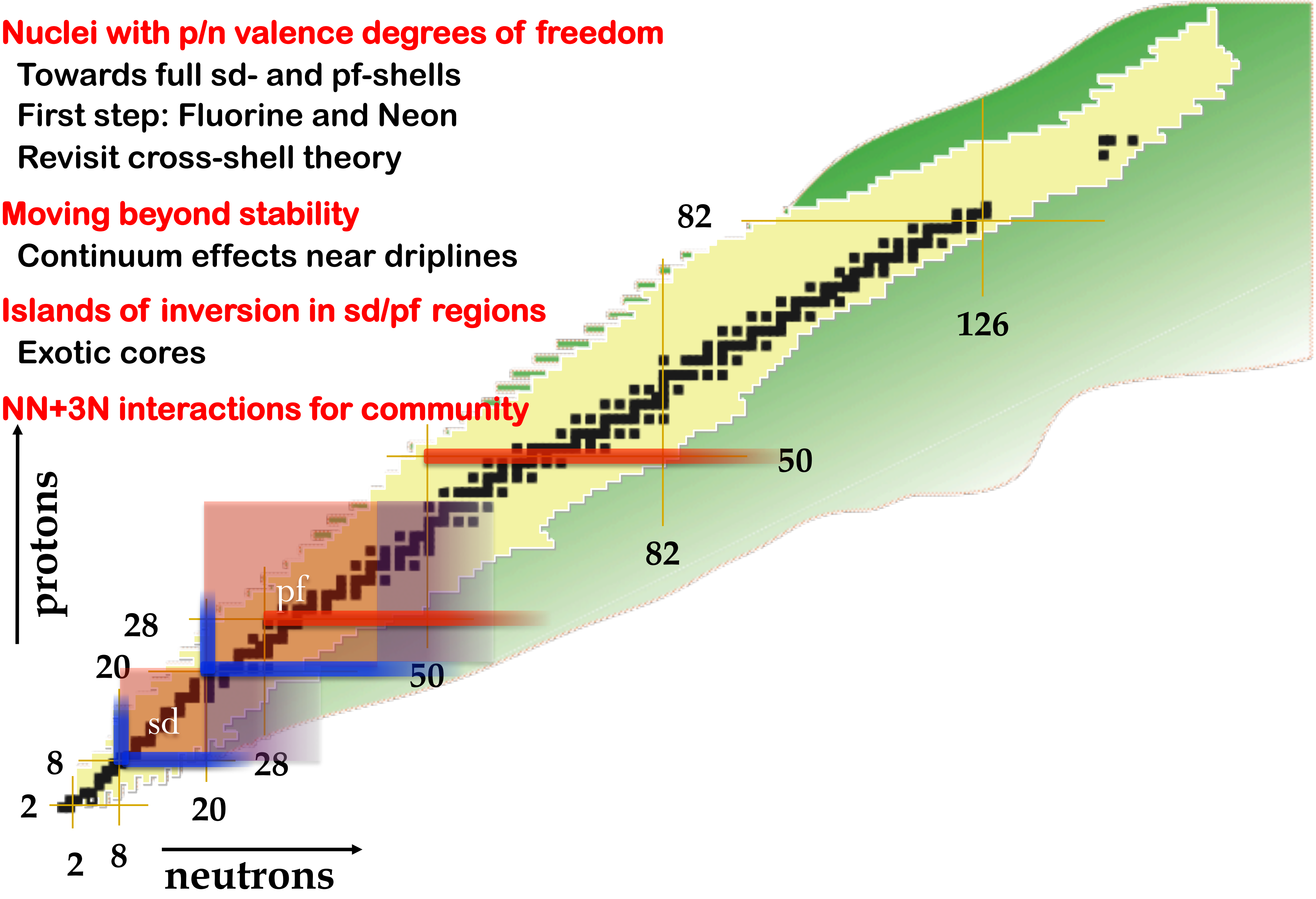
Moving beyond stability

Continuum effects near driplines

Islands of inversion in sd/pf regions

Exotic cores

NN+3N interactions for community



New Directions and Outlook

Heavier semi-magic chains: Nickel and Tin

Nuclei with p/n valence degrees of freedom

Towards full sd- and pf-shells

First step: Fluorine and Neon

Revisit cross-shell theory

Moving beyond stability

Continuum effects near driplines

Islands of inversion in sd/pf regions

Exotic cores

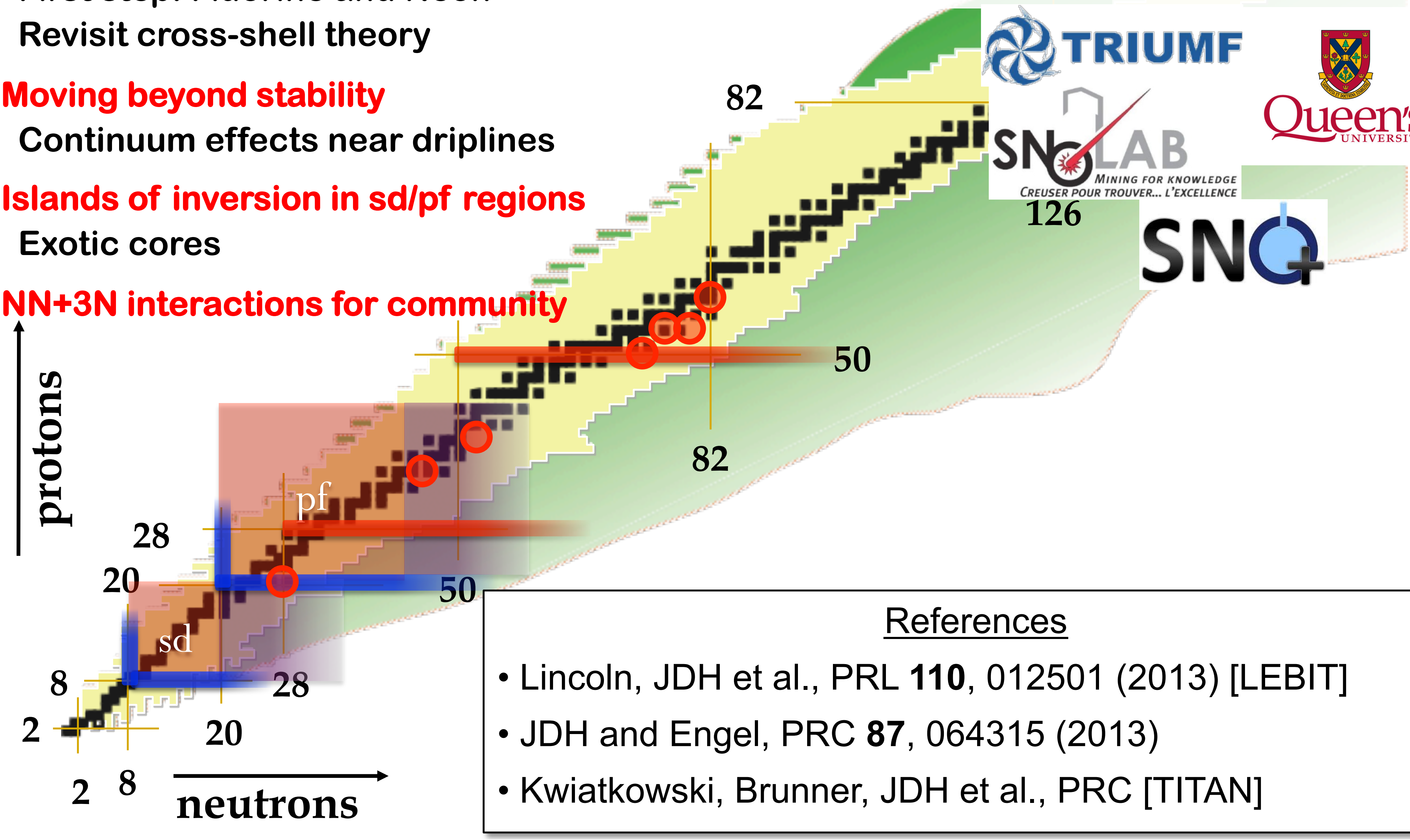
NN+3N interactions for community

Fundamental symmetries

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

Effective electroweak operators

WIMP-nucleus scattering

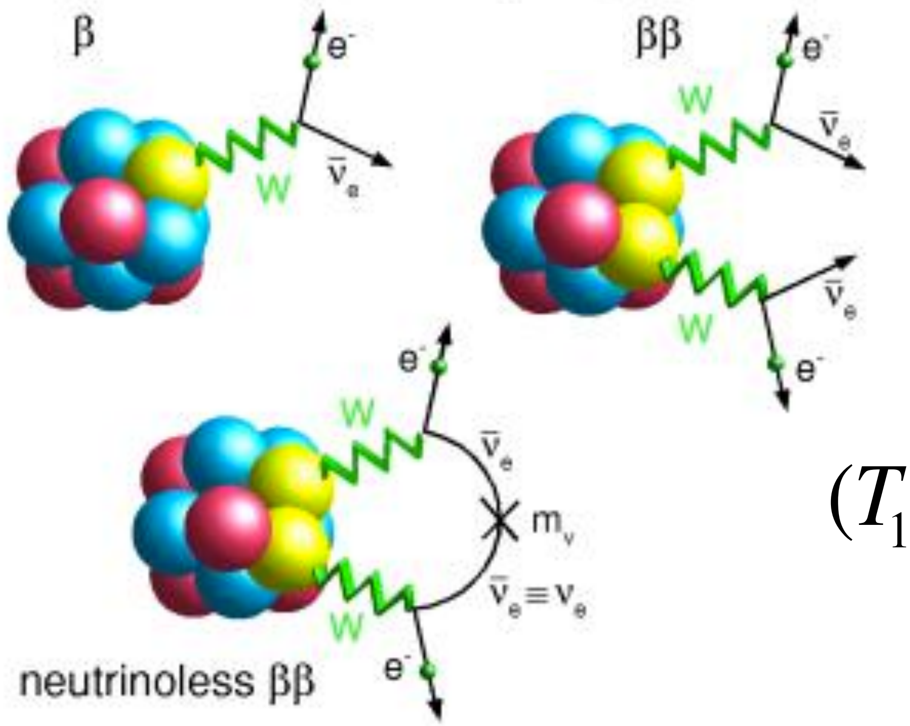


References

- Lincoln, JDH et al., PRL **110**, 012501 (2013) [LEBIT]
- JDH and Engel, PRC **87**, 064315 (2013)
- Kwiatkowski, Brunner, JDH et al., PRC [TITAN]

Fundamental Symmetries: 0νββ-Decay

What is the nature and mass of the neutrino?



Two essential ingredients:

Q-value (experiment)

Nuclear matrix element

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

$$M_{0\nu} = \left\langle f \left| M_{0\nu}^{GT} - \frac{g_v^2}{g_A^2} M_{0\nu}^{F} + \cdots \right| i \right\rangle$$

Calculations of $M_{0\nu}$ in ^{48}Ca, ^{76}Ge, and ^{82}Se

Phenomenological wavefunctions from A. Poves, M. Horoi

^{48}Ca	Bare	**0.77**
	Effective	**1.30**

^{76}Ge	Bare	**3.12**
	Effective	**3.77**

^{82}Se	Bare	**2.73**
	Effective	**3.62**

Converged in 13 major oscillator shells

Lincoln, JDH et al. [LEBIT], PRL (2013)

JDH and Engel, PRC (2013)

Kwiatkowski, Brunner, JDH et al. [TITAN], PRC (2014)

Overall ~25-30% increase for ^{76}Ge, ^{82}Se; 75% for ^{48}Ca

Promising first steps – up next…

- Consistent wavefunctions and operators from NN+3N
- Improve operator: 2-body currents from chiral EFT
- Non-perturbative methods (IM-SRG)
- Effects of induced 3-body operators

Menendez, Gazit, Schwenk, PRL (2011)

Shukla, Engel, Navratil, PRC (2011)

New Directions and Outlook

Heavier semi-magic chains: Nickel and Tin

Nuclei with p/n valence degrees of freedom

Towards full sd- and pf-shells
First step: Fluorine and Neon
Revisit cross-shell theory

Moving beyond stability

Continuum effects near driplines

Islands of inversion in sd/pf regions

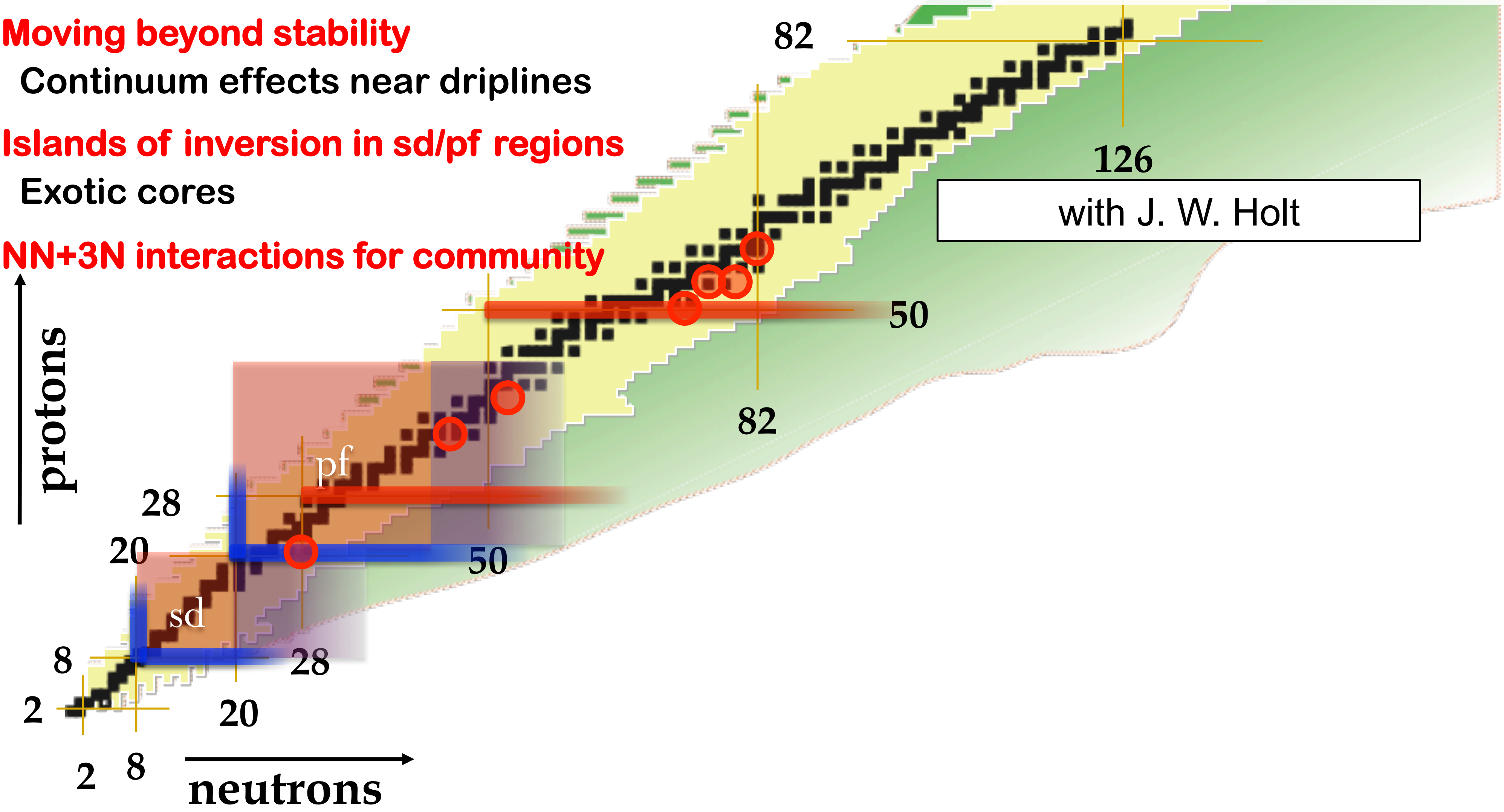
Exotic cores

NN+3N interactions for community

Fundamental symmetries

Non-empirical calculation of $0\nu\beta\beta$ decay
Effective electroweak operators
WIMP-nucleus scattering

Ab-initio optical model potential



with J. W. Holt

New Directions and Outlook

Heavier semi-magic chains: Nickel and Tin

Nuclei with p/n valence degrees of freedom

Towards full sd- and pf-shells

First step: Fluorine and Neon

Revisit cross-shell theory

Moving beyond stability

Continuum effects near driplines

Islands of inversion in sd/pf regions

Exotic cores

NN+3N interactions for community

Fundamental symmetries

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

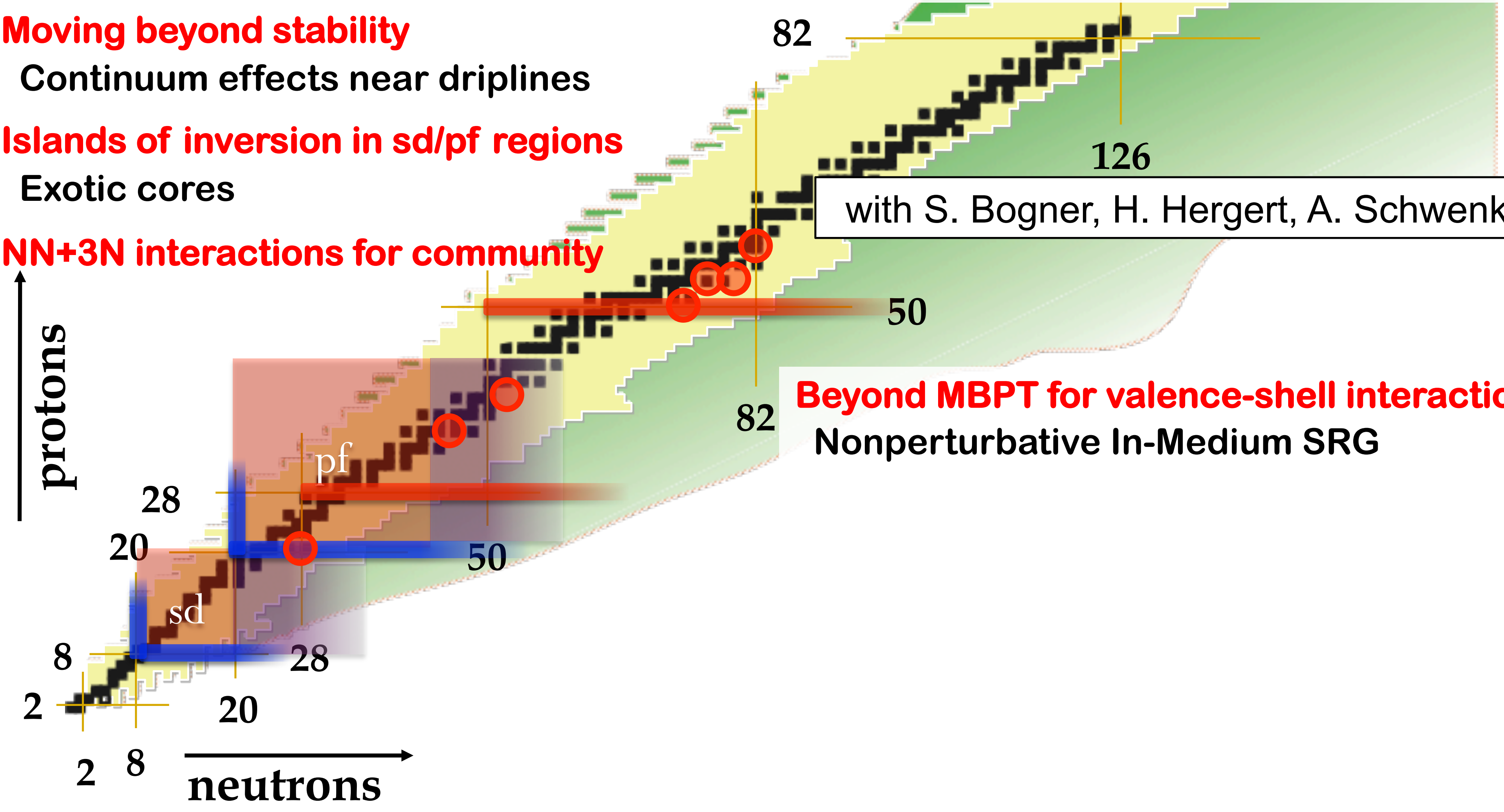
Effective electroweak operators

WIMP-nucleus scattering

Ab-initio optical model potential

Beyond MBPT for valence-shell interactions

Nonperturbative In-Medium SRG



with S. Bogner, H. Hergert, A. Schwenk

New Directions and Outlook

Heavier semi-magic chains: Nickel and Tin

Nuclei with p/n valence degrees of freedom

Towards full sd- and pf-shells

First step: Fluorine and Neon

Revisit cross-shell theory

Moving beyond stability

Continuum effects near driplines

Islands of inversion in sd/pf regions

Exotic cores

NN+3N interactions for community

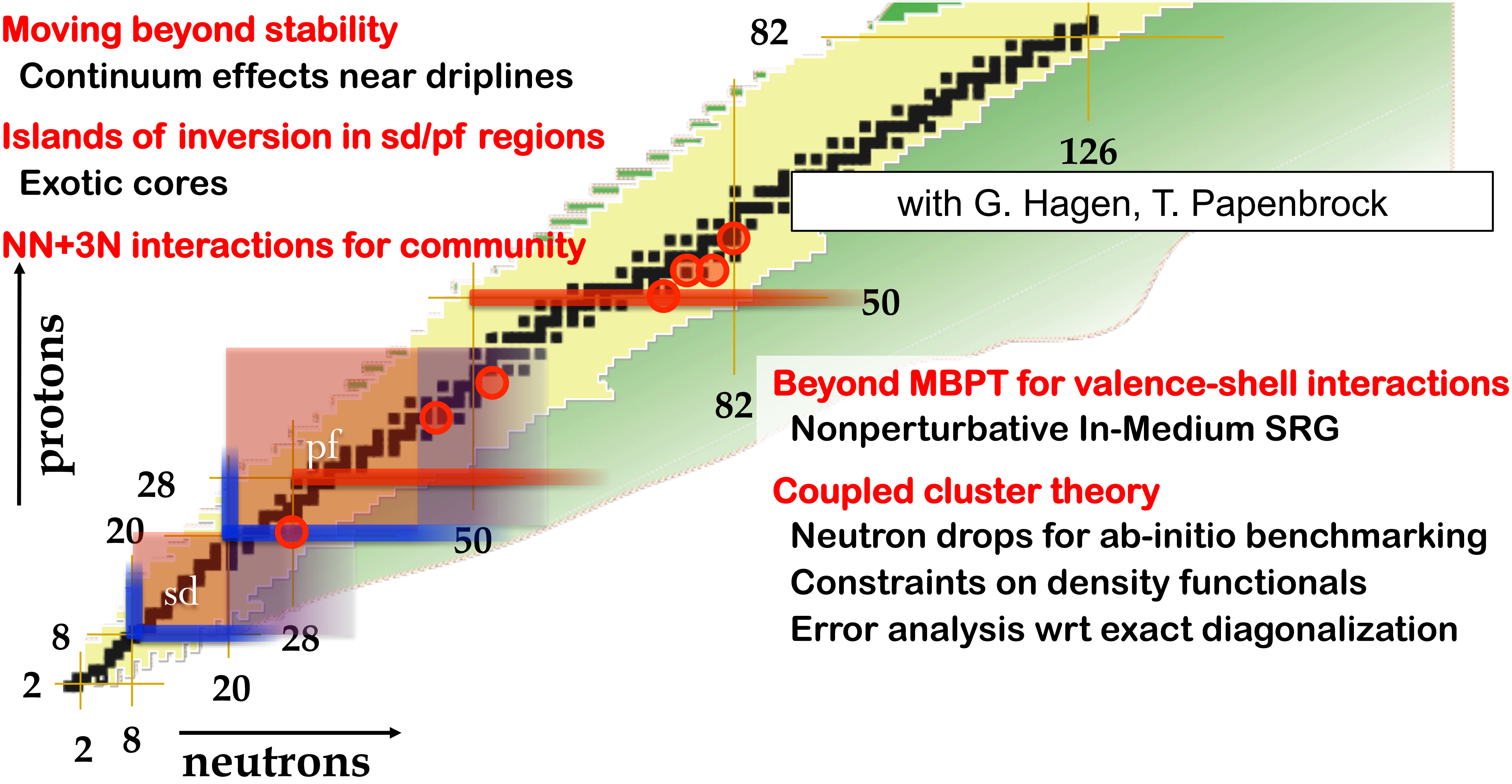
Fundamental symmetries

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

Effective electroweak operators

WIMP-nucleus scattering

Ab-initio optical model potential



Beyond MBPT for valence-shell interactions

Nonperturbative In-Medium SRG

Coupled cluster theory

Neutron drops for ab-initio benchmarking

Constraints on density functionals

Error analysis wrt exact diagonalization

New Directions and Outlook

Heavier semi-magic chains: Nickel and Tin

Nuclei with p/n valence degrees of freedom

Towards full sd- and pf-shells
First step: Fluorine and Neon
Revisit cross-shell theory

Moving beyond stability

Continuum effects near driplines

Islands of inversion in sd/pf regions

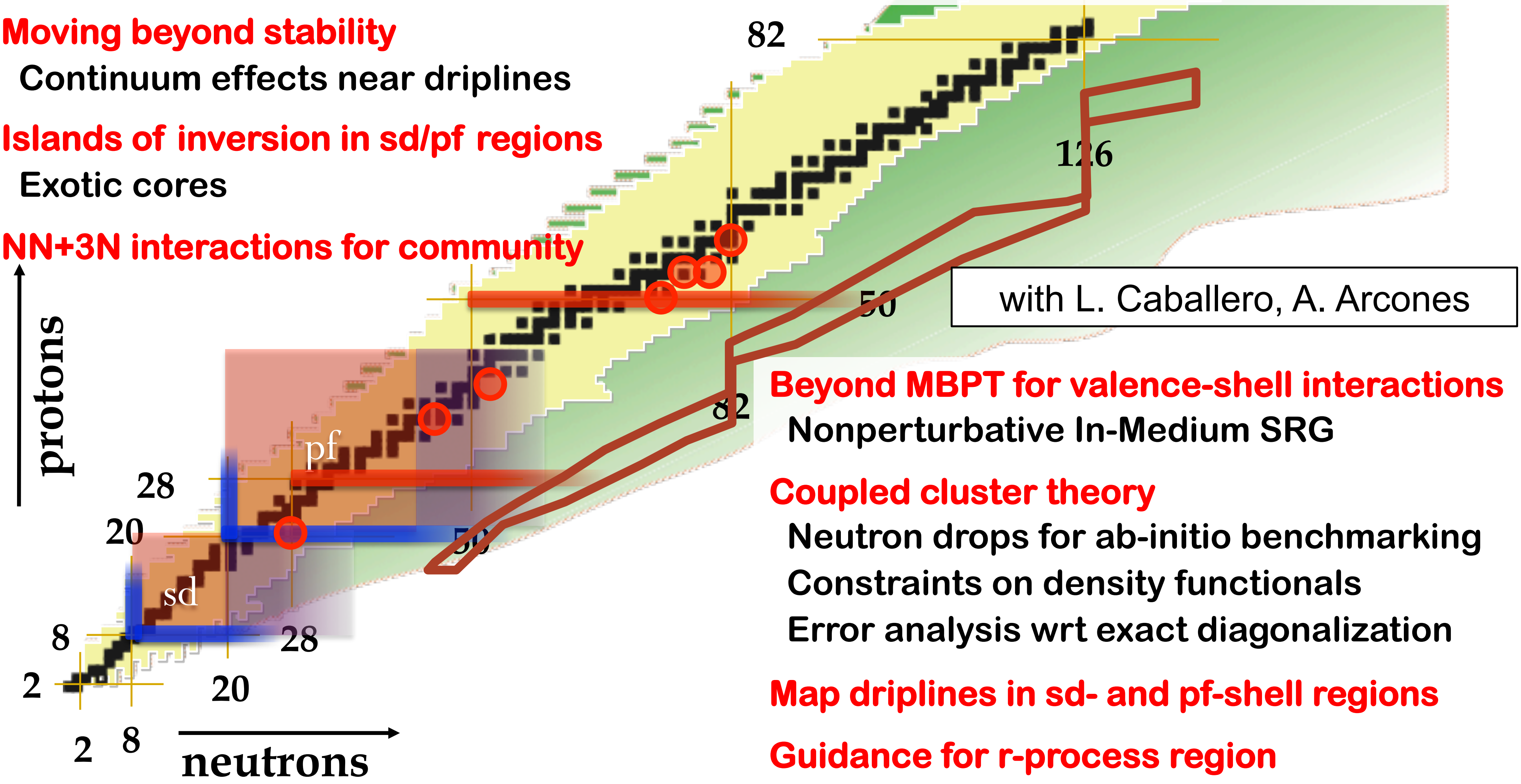
Exotic cores

NN+3N interactions for community

Fundamental symmetries

Non-empirical calculation of $0\nu\beta\beta$ decay
Effective electroweak operators
WIMP-nucleus scattering

Ab-initio optical model potential



with L. Caballero, A. Arcones

Beyond MBPT for valence-shell interactions

Nonperturbative In-Medium SRG

Coupled cluster theory

Neutron drops for ab-initio benchmarking
Constraints on density functionals
Error analysis wrt exact diagonalization

Map driplines in sd- and pf-shell regions

Guidance for r-process region

New Directions and Outlook

Heavier semi-magic chains: Nickel and Tin

Nuclei with p/n valence degrees of freedom

Towards full sd- and pf-shells

First step: Fluorine and Neon

Revisit cross-shell theory

Moving beyond stability

Continuum effects near driplines

Islands of inversion in sd/pf regions

Exotic cores

NN+3N interactions for community

Fundamental symmetries

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

Effective electroweak operators

WIMP-nucleus scattering

Ab-initio optical model potential

Beyond MBPT for valence-shell interactions

Nonperturbative In-Medium SRG

Coupled cluster theory

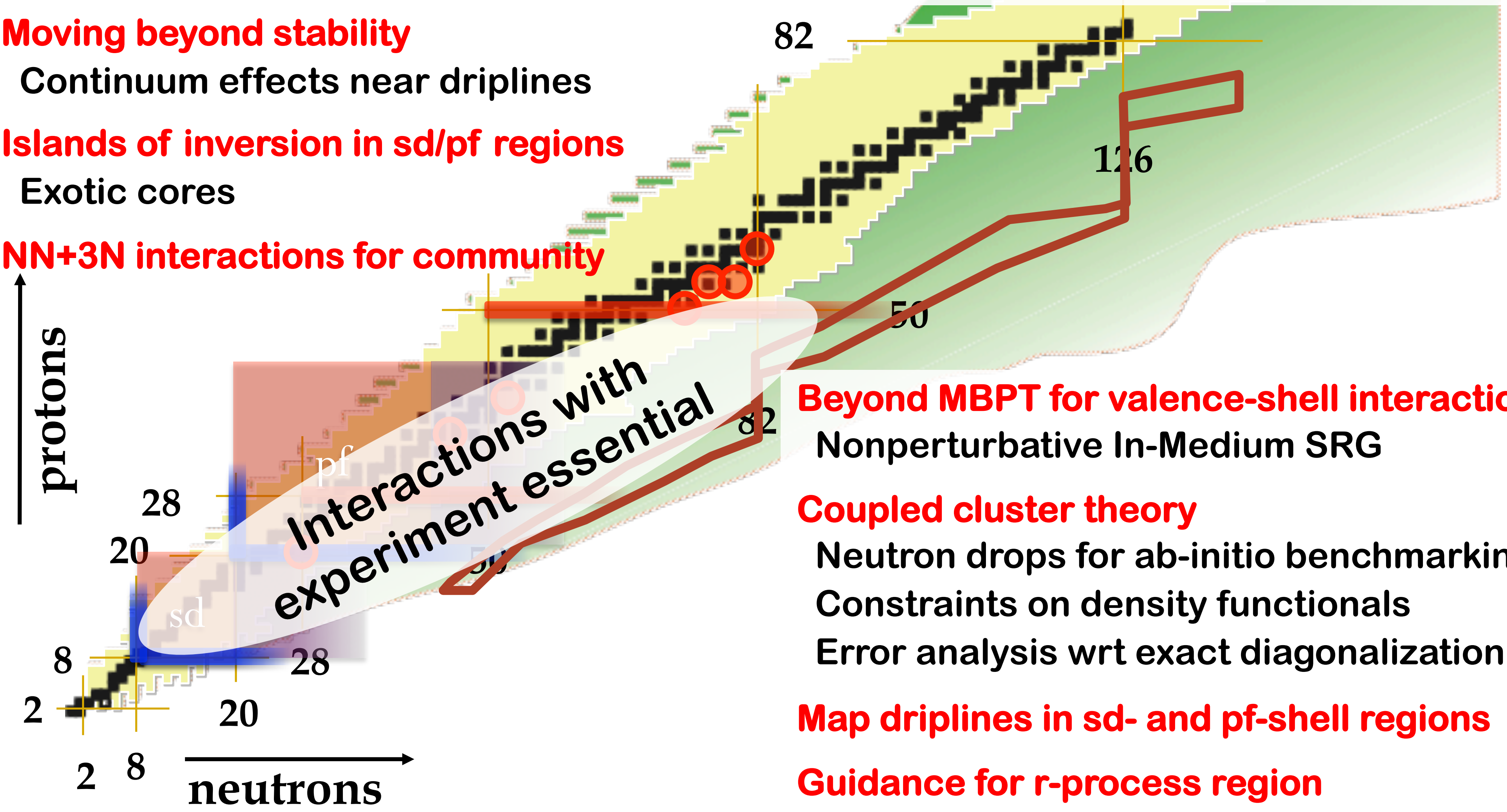
Neutron drops for ab-initio benchmarking

Constraints on density functionals

Error analysis wrt exact diagonalization

Map driplines in sd- and pf-shell regions

Guidance for r-process region



Interactions with experiment essential

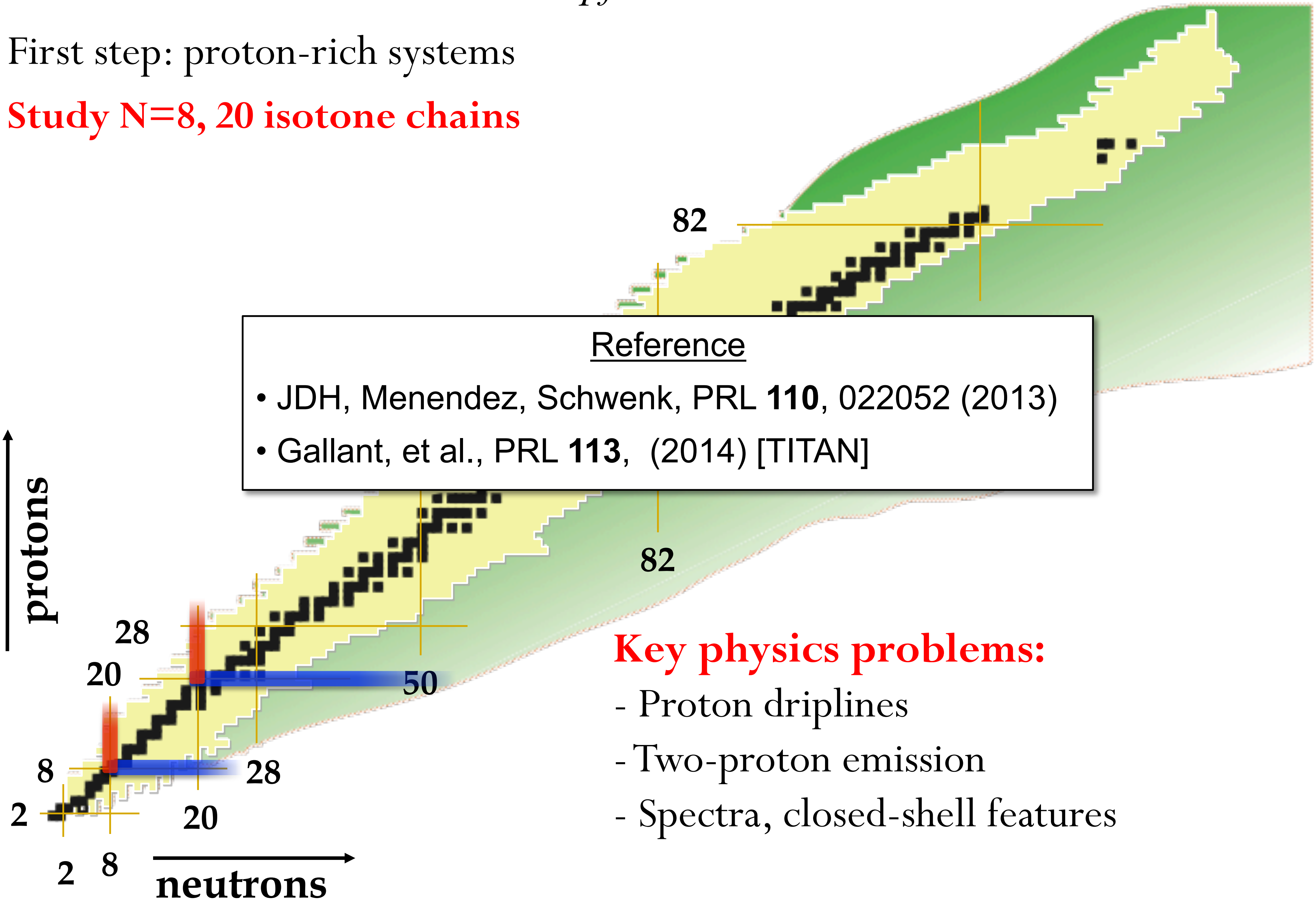
Proton Dripline

Proton-Rich Systems

Towards calculations of all *sd*- and *pf*-shell nuclei: islands of inversion

First step: proton-rich systems

Study N=8, 20 isotone chains



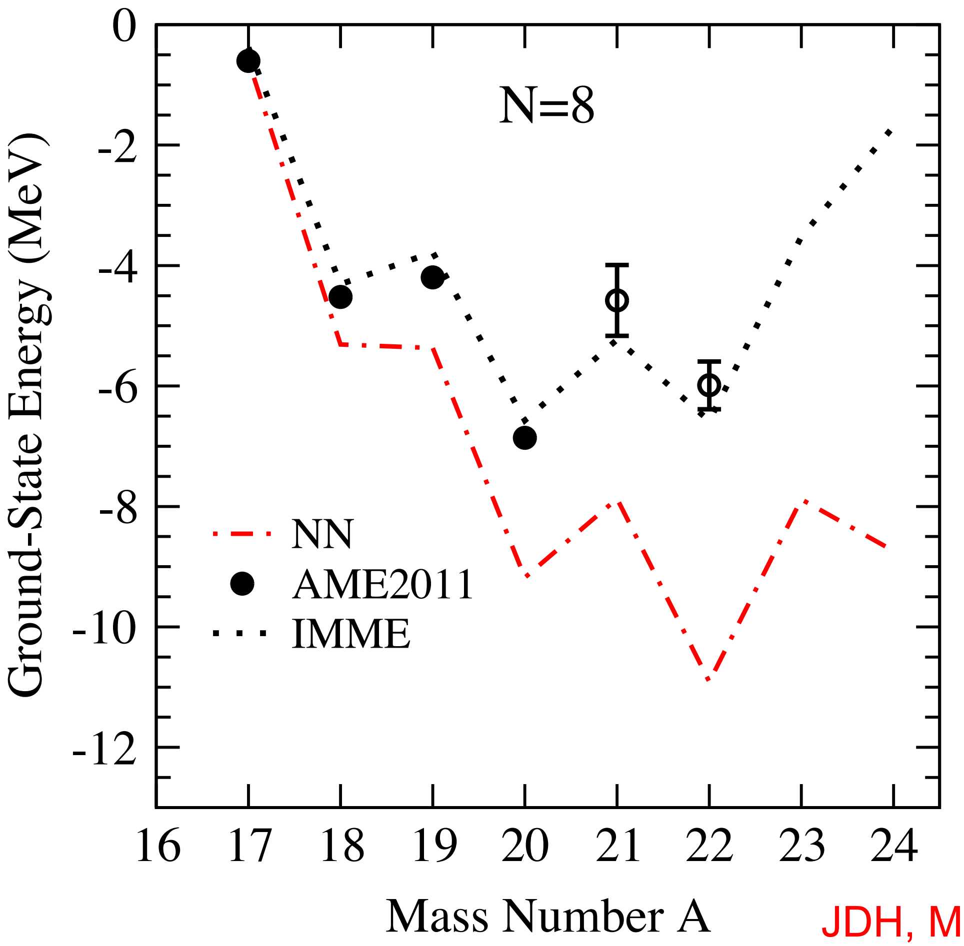
Reference

- JDH, Menendez, Schwenk, PRL **110**, 022052 (2013)
- Gallant, et al., PRL **113**, (2014) [TITAN]

Key physics problems:

- Proton driplines
- Two-proton emission
- Spectra, closed-shell features

Ground-State Energies of N=8 Isotones



Data limited – use phenomenological isobaric multiplet mass equation (IMME)

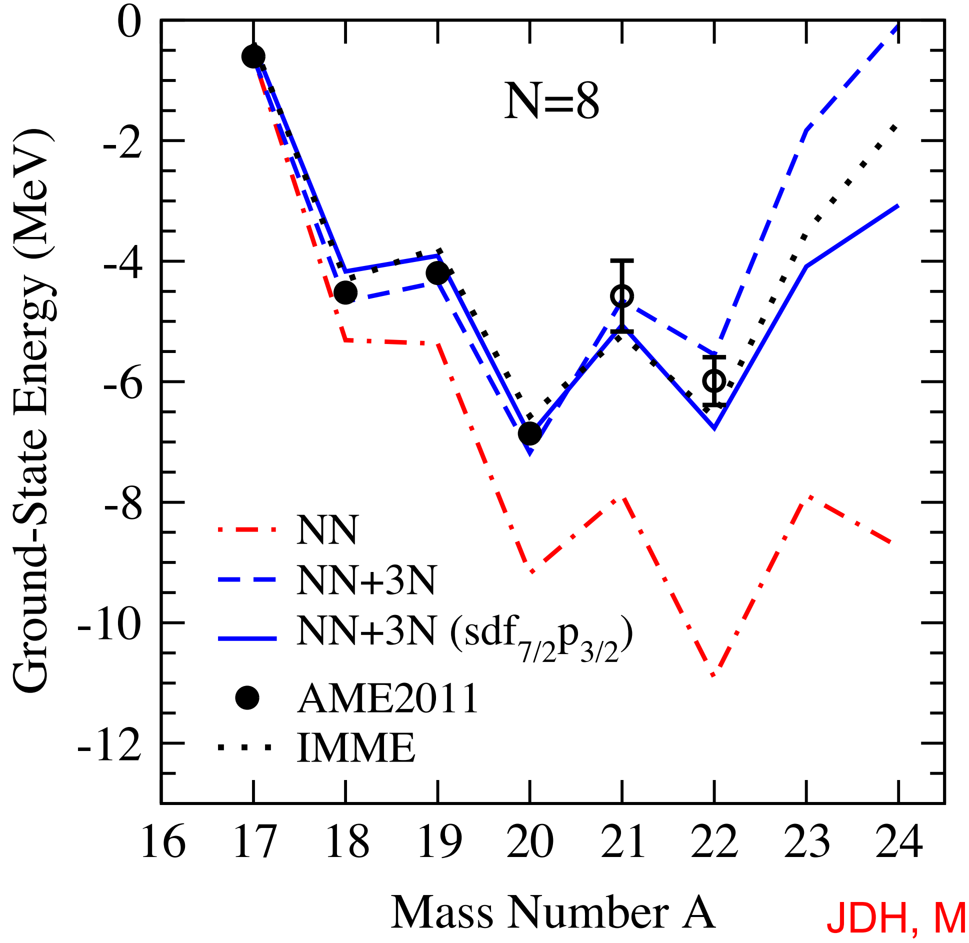
$$E(A,T,T_z) = E(A,T,-T_z) + 2b(A,T)T_z$$

$$b = 0.7068A^{2/3} - 0.9133$$

NN-only: overbound

JDH, Menendez, Schwenk, PRL (2013)

Ground-State Energies of N=8 Isotones



Data limited – use phenomenological isobaric multiplet mass equation (IMME)

$$E(A,T,T_z) = E(A,T,-T_z) + 2b(A,T)T_z$$

$$b = 0.7068A^{2/3} - 0.9133$$

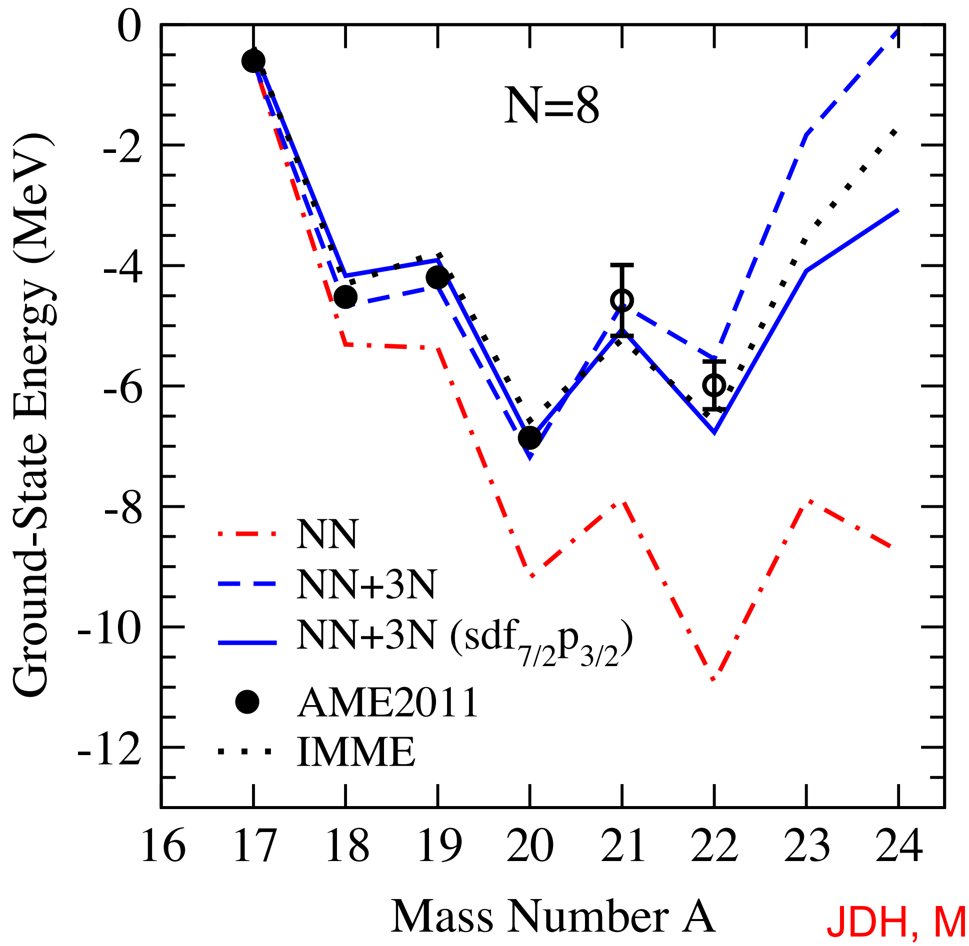
NN-only: overbound

NN+3N: improved agreement with experiment/IMME

JDH, Menendez, Schwenk, PRL (2013)

Dripline unclear: ^{22}Si unbound in AME, NN+3N; bound in IMME

Ground-State Energies of N=8 Isotones



JDH, Menendez, Schwenk, PRL (2013)

Data limited – use phenomenological isobaric multiplet mass equation (IMME)

$$E(A,T,T_z) = E(A,T,-T_z) + 2b(A,T)T_z$$

$$b = 0.7068A^{2/3} - 0.9133$$

NN-only: overbound

NN+3N: improved agreement with experiment/IMME

Dripline unclear: ^{22}Si unbound in AME, NN+3N; bound in IMME

^{22}**Si** possible two-proton emitter

Mass measurement needed!

	IMME	**NN+3N (*sd*)**	**NN+3N (*$sdf_{7/2}p_{3/2}$*)**
S_{2p}	0.01 MeV	-1.63 MeV	-0.12 MeV

N=8 and N=20 Proton SPEs

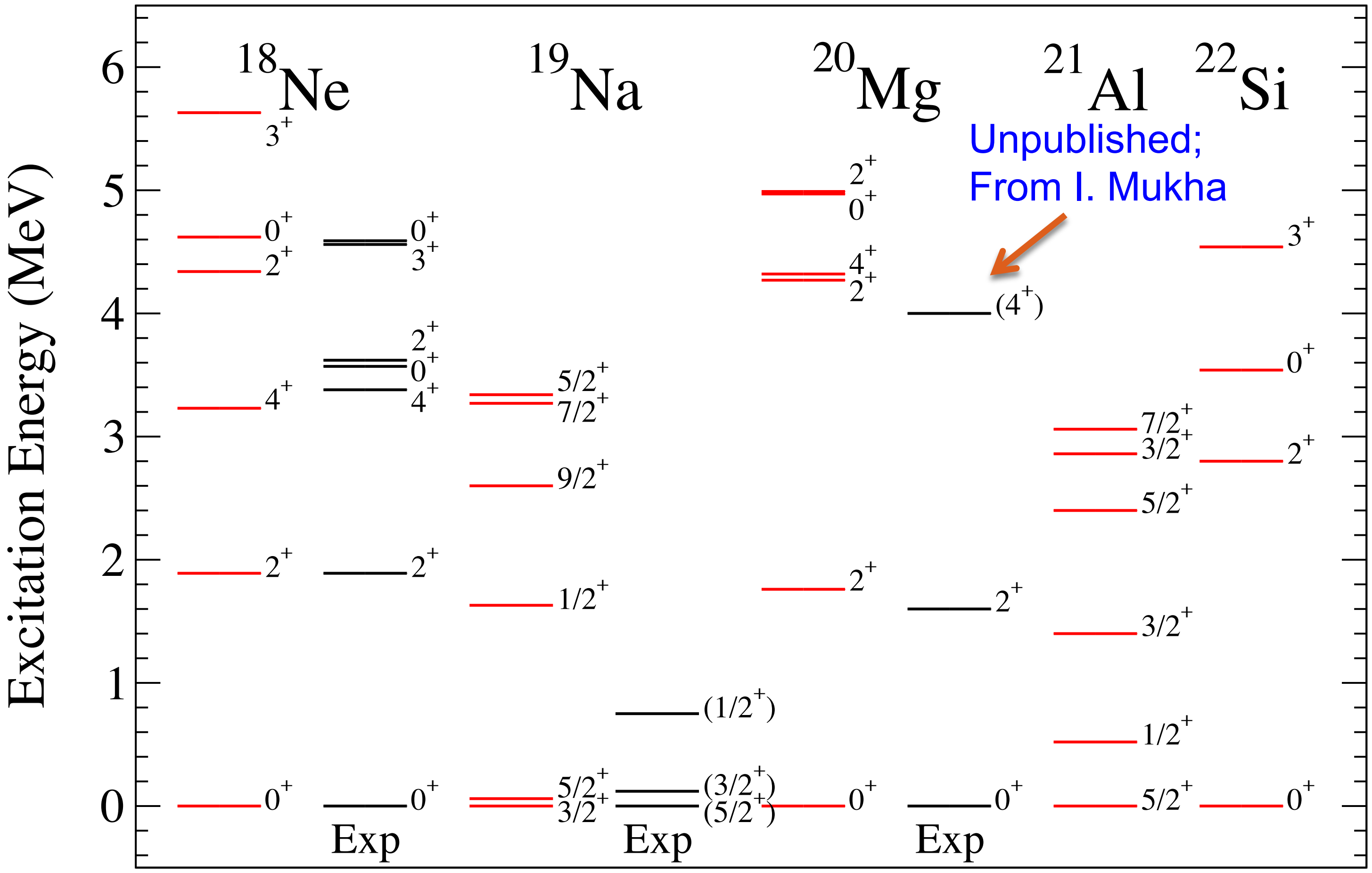
Interaction and self-consistent SPEs from NN+3N $sdf_{7/2}p_{3/2}$- and $pfg_{9/2}$-spaces

NN-only: empirical SPEs in *sd*- and *pf*-shells only

Orbit	Empirical	$T+V_{NN}+V_{3N}$
$d_{5/2}$	-0.60	-0.41
$s_{1/2}$	-0.10	0.95
$d_{3/2}$	4.40	4.57
$f_{7/2}$	-	9.73
$p_{3/2}$	-	12.64

Orbit	Empirical	$T+V_{NN}+V_{3N}$
$f_{7/2}$	-1.07	-0.86
$p_{3/2}$	-0.63	1.40
$p_{1/2}$	2.38	3.94
$f_{5/2}$	5.00	5.36
$g_{9/2}$	-	6.40

Spectra of N=8 Isotones



Unpublished;
From I. Mukha

JDH, Menendez, Schwenk, PRL (2012)

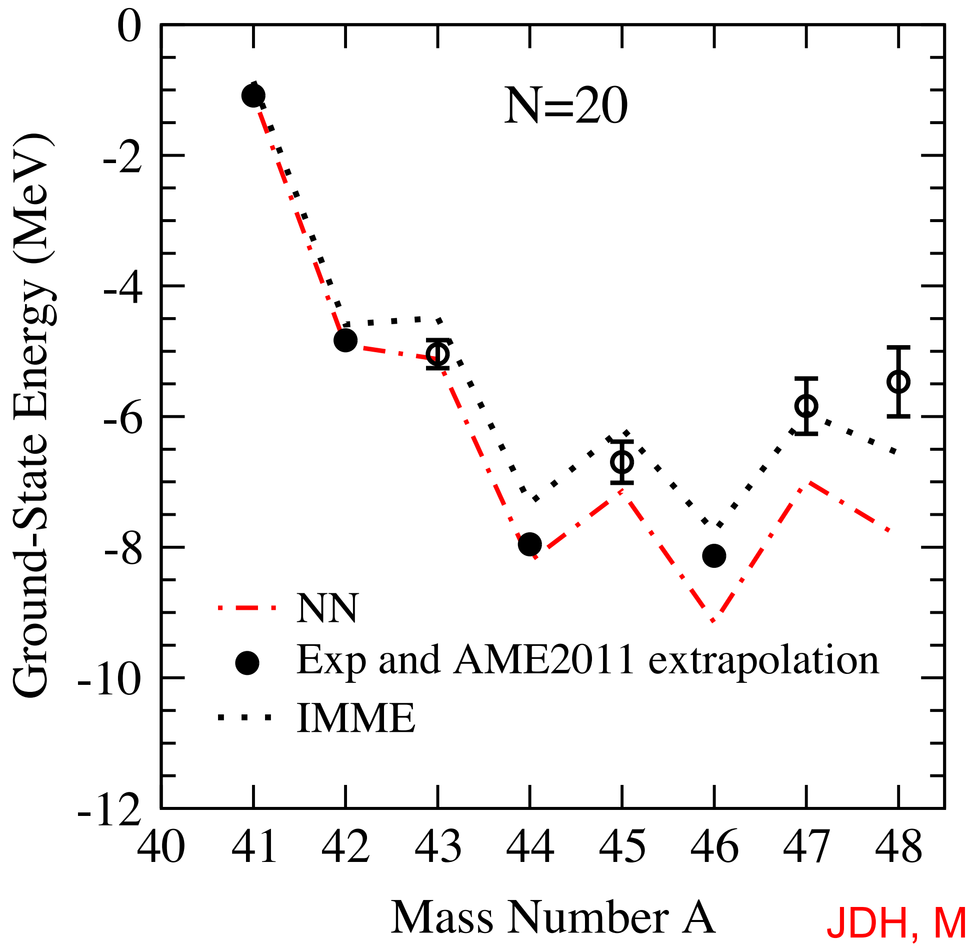
NN+3N: reasonable agreement with experiment

New measurement: excited state in ^{20}Mg close to predicted 4^+-2^+ doublet

Predictions for proton-rich ^{21}Al, ^{22}Si spectra

Closed sub-shell signature in ^{22}Si

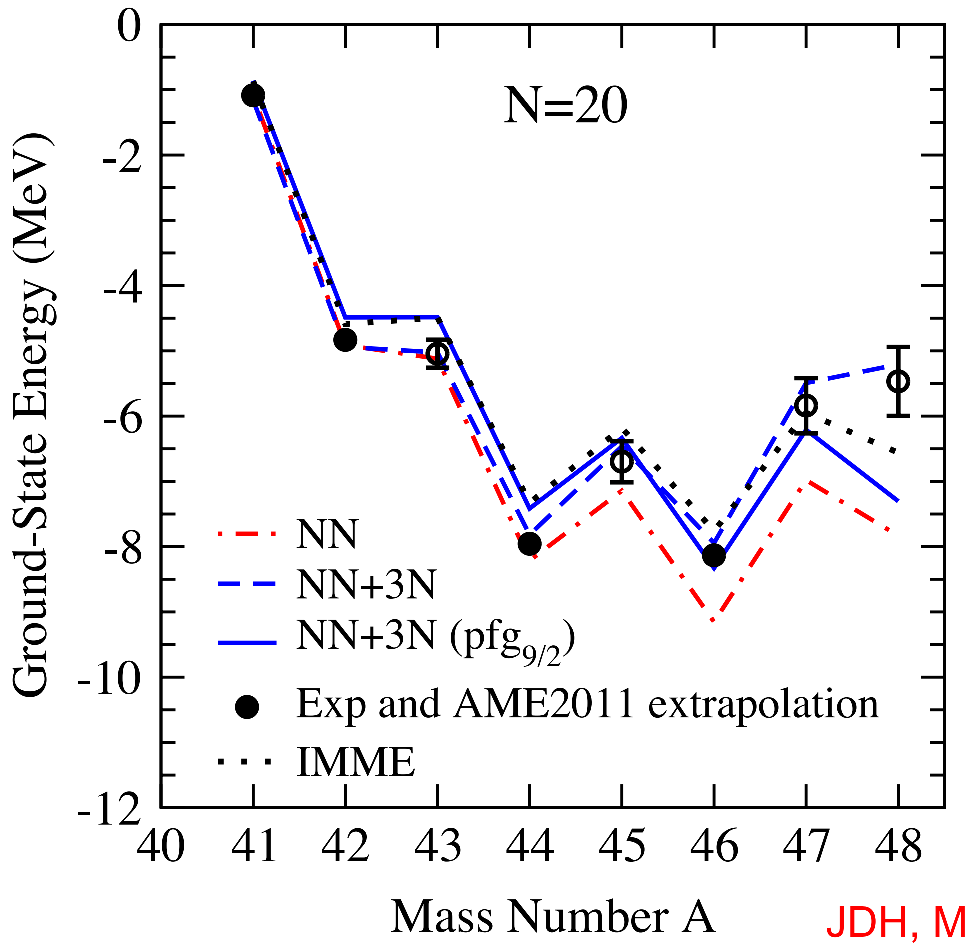
Ground-State Energies of N=20 Isotones



NN-only: overbound beyond ^{45}Mn

JDH, Menendez, Schwenk, PRL (2013)

Ground-State Energies of N=20 Isotones



NN-only: overbound beyond ^{45}Mn

NN+3N: close to experiment/IMME

JDH, Menendez, Schwenk, PRL (2013)

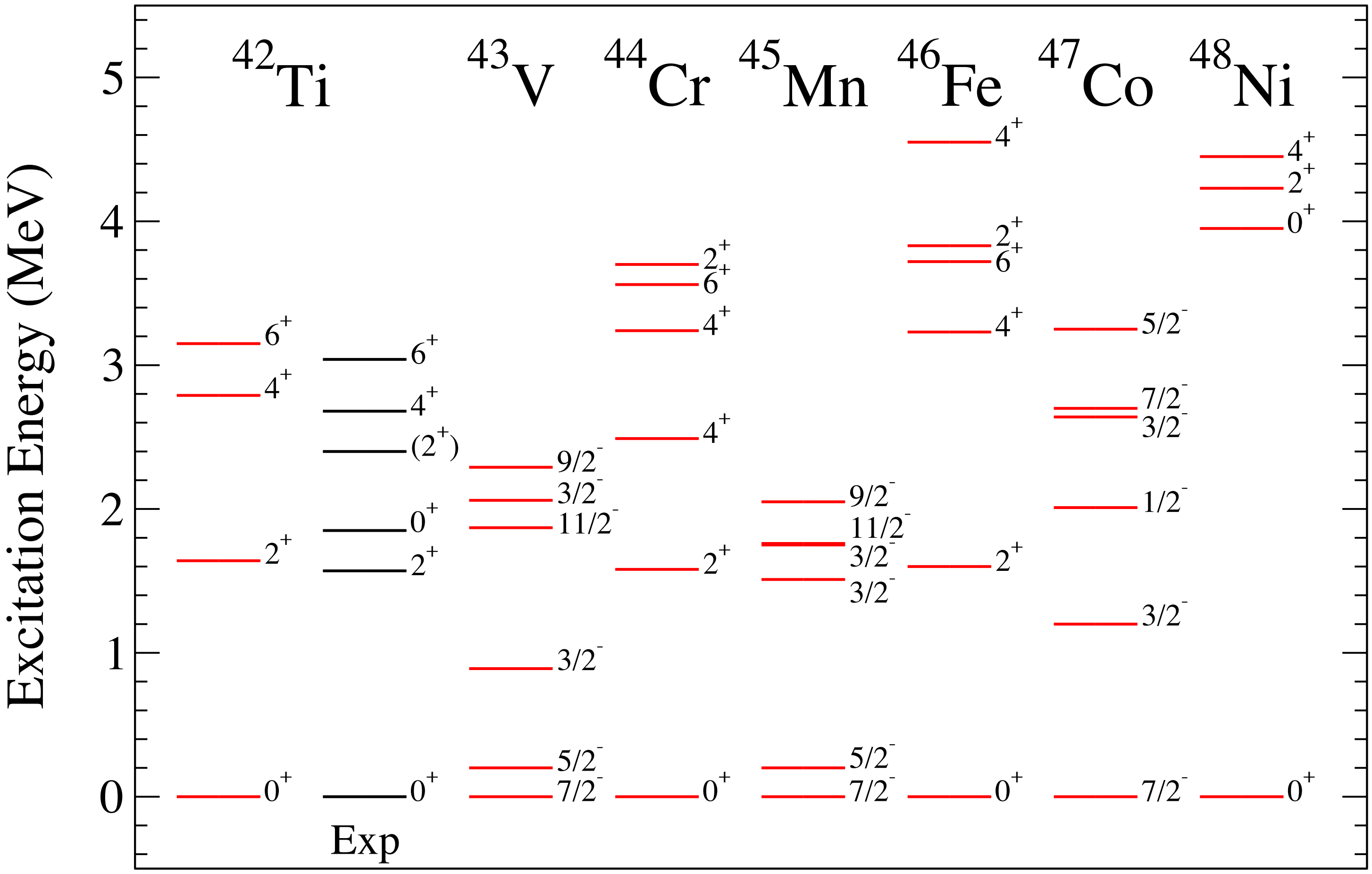
Dripline: Predicted to be ^{46}Fe in all calculations

S_{2p}	**Expt.**	**NN+3N (*pf*)**	**NN+3N (*pfg*$_{9/2}$)**
	-1.28(6) MeV	-2.73 MeV	-1.02 MeV

Prediction for ^{48}Ni within 300keV of experiment

Dossat et al (2005); Pomorski et al (2012)

Spectra of N=20 Isotones



JDH, Menendez, Schwenk, PRL (2013)

NN+3N: reasonable agreement with measured ^{42}Ti

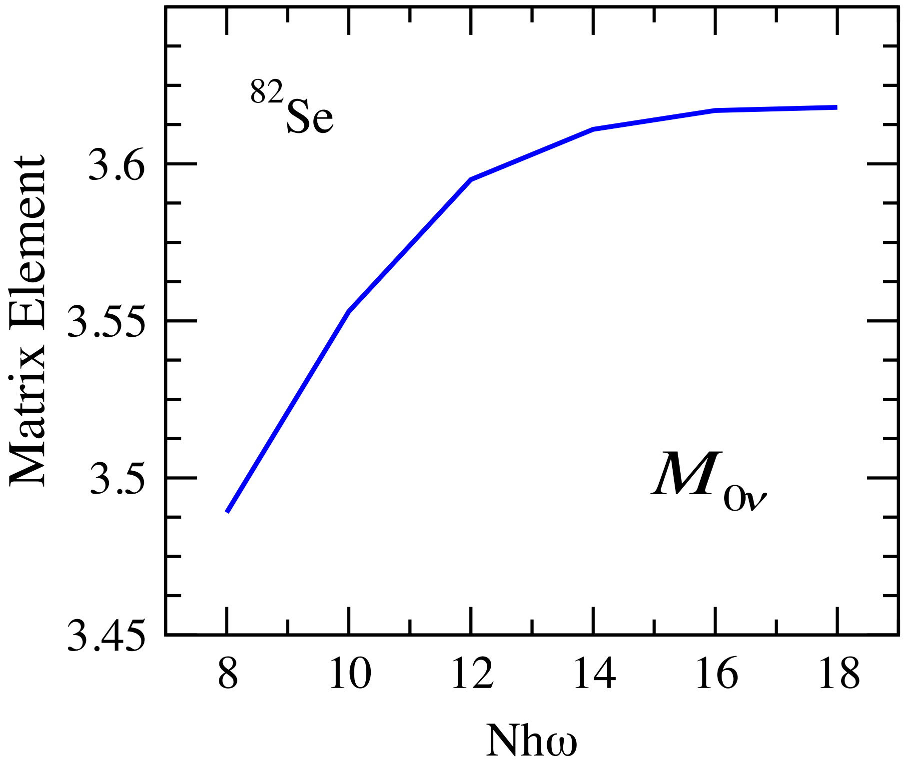
Predictions for proton-rich spectra

Mirror energy differences with Ca isotopes ~400keV

Closed-shell signature in ^{48}Ni

Intermediate-State Convergence

Results in ^{82}Se (with phenomenological wavefunctions from A. Poves)



JDH and Engel, PRC (2013)

Results **well converged** in terms of intermediate state excitations

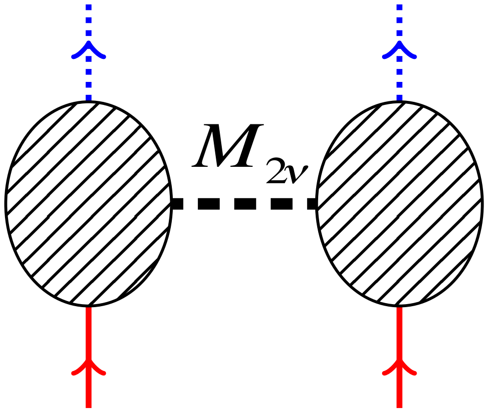
Improvement due to low-momentum interactions

Similar trend in ^{76}Ge and ^{48}Ca

Quenching of GT Strength

Investigate many-body effects on quenching of g_A

Set of two-body diagrams contributing to renormalization of g_A in 2νββ decay: product of 2 single-beta-decay

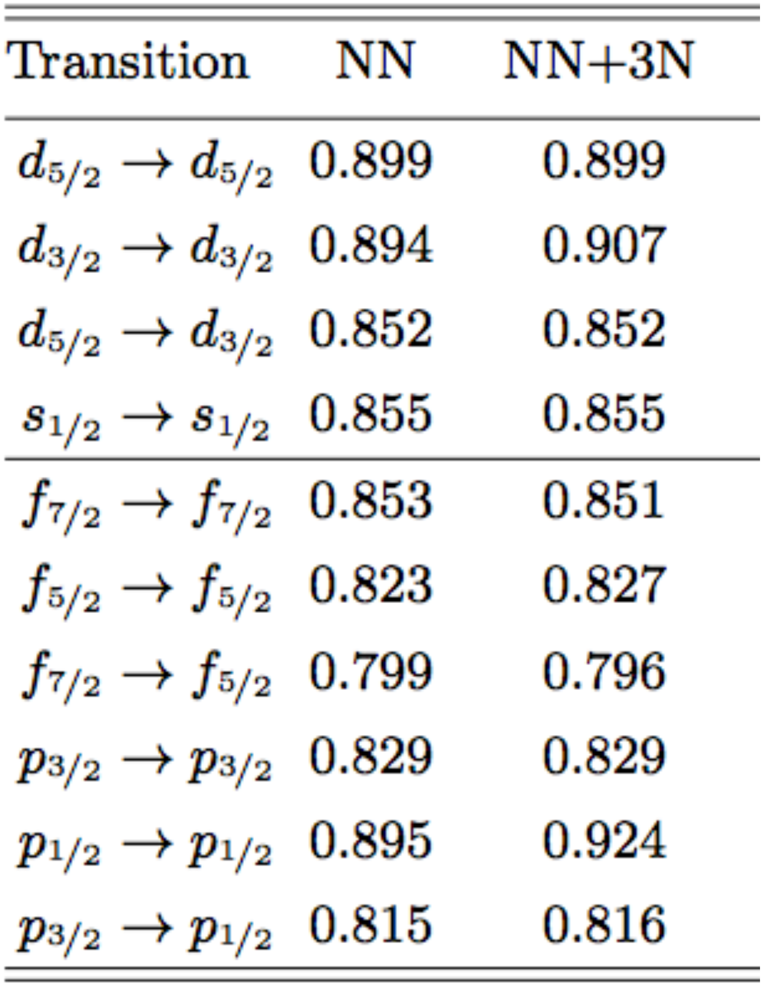


Quenching of 38% in ^{82}Se ($g_A \sim 1.0$)

Quenching of GT Strength

Investigate many-body effects on quenching of g_A

Calculate GT transitions in sd- and pf-shells



Transition	NN	NN+3N
$d_{5/2} \to d_{5/2}$	0.899	0.899
$d_{3/2} \to d_{3/2}$	0.894	0.907
$d_{5/2} \to d_{3/2}$	0.852	0.852
$s_{1/2} \to s_{1/2}$	0.855	0.855
$f_{7/2} \to f_{7/2}$	0.853	0.851
$f_{5/2} \to f_{5/2}$	0.823	0.827
$f_{7/2} \to f_{5/2}$	0.799	0.796
$p_{3/2} \to p_{3/2}$	0.829	0.829
$p_{1/2} \to p_{1/2}$	0.895	0.924
$p_{3/2} \to p_{1/2}$	0.815	0.816

Net quenching between 0.8-0.9

Consistent with findings from $2\nu\beta\beta$ decay

Larger quenching when spin-orbit partners absent from valence space

Converged using low-momentum interactions – little effect from 3N

Backup Details

Renormalization of Nuclear Interactions

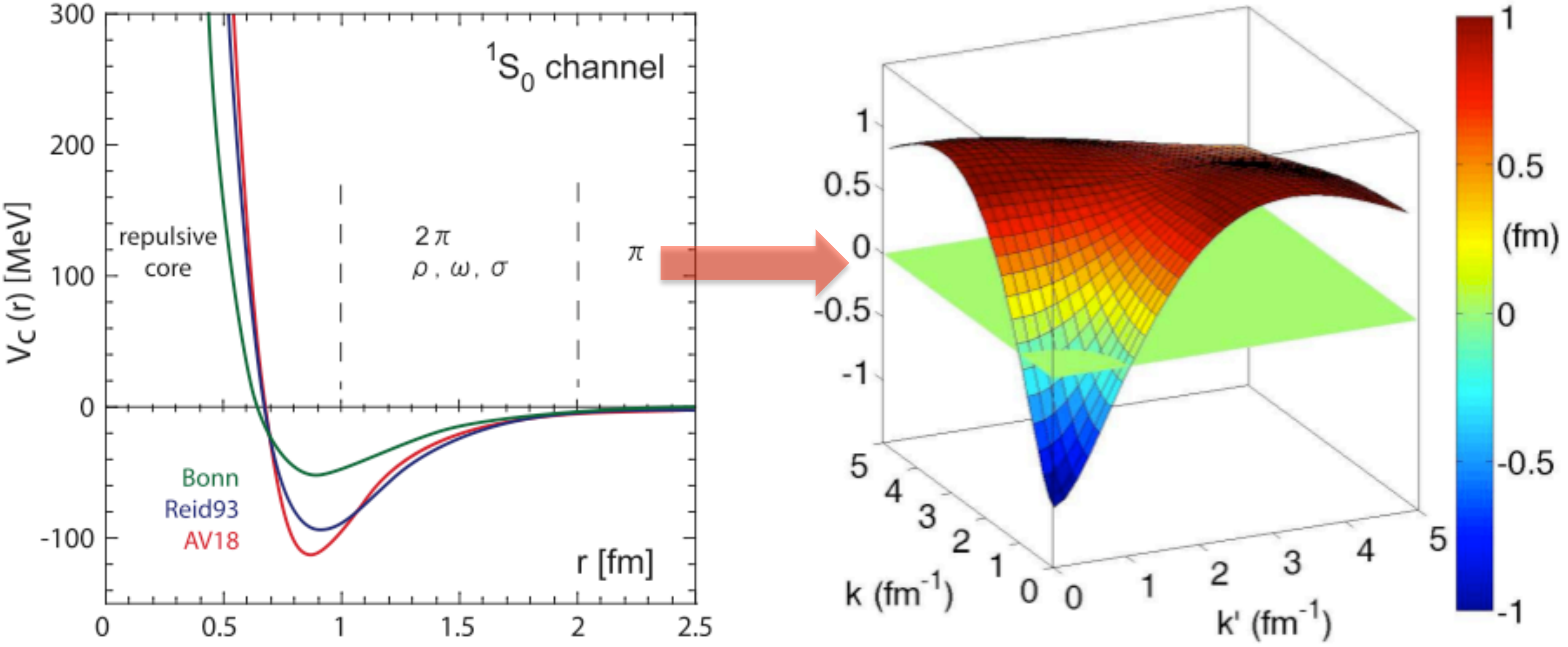
$$H(\Lambda) = T + V_{\mathrm{NN}}(\Lambda) + V_{3\mathrm{N}}(\Lambda) + V_{4\mathrm{N}}(\Lambda) + \ldots$$

Textbook nuclear potentials in **r**-space

- Hard core, long-range one-pion exchange

Also treat in momentum space

- Strong high-momentum repulsion, coupling of low to high momenta



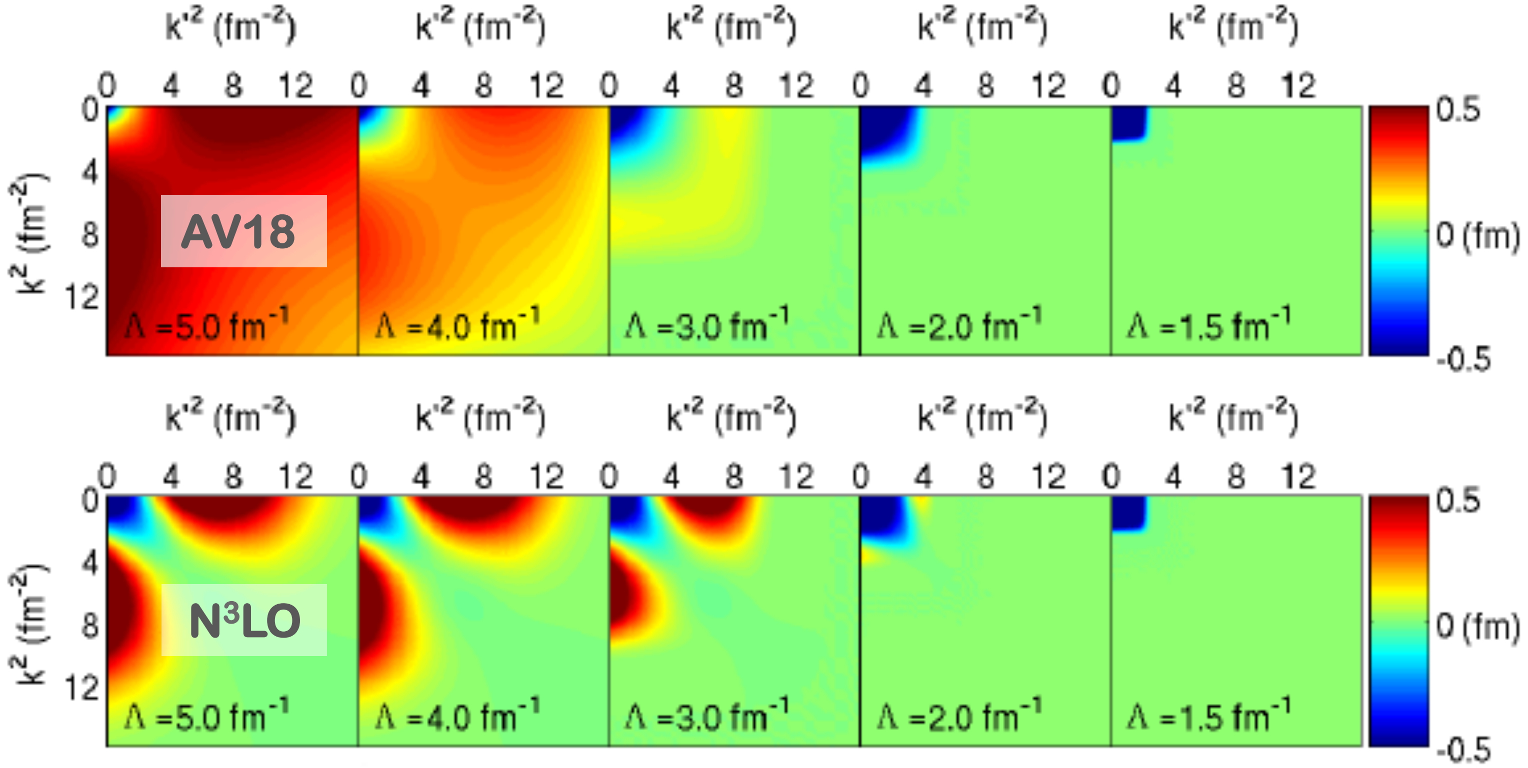
Renormalization of Nuclear Interactions

$$\boxed{H(\Lambda) = T + V_{\mathrm{NN}}(\Lambda) + V_{3\mathrm{N}}(\Lambda) + V_{4\mathrm{N}}(\Lambda) + \ldots}$$

Evolve momentum resolution scale of chiral interactions from initial Λ_χ

Remove coupling to high momenta, low-energy physics unchanged

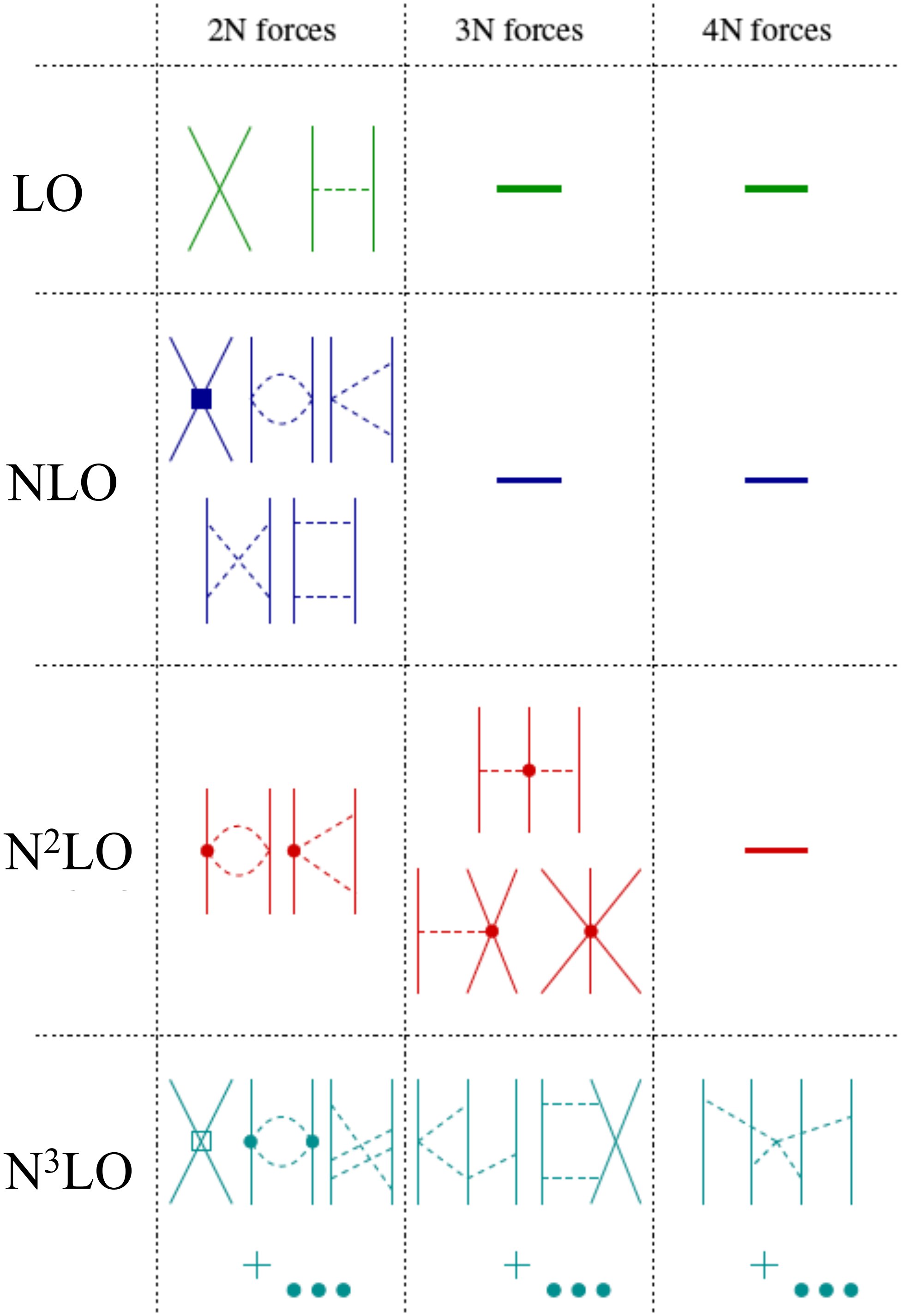
Bogner, Kuo, Schwenk, Furnstahl



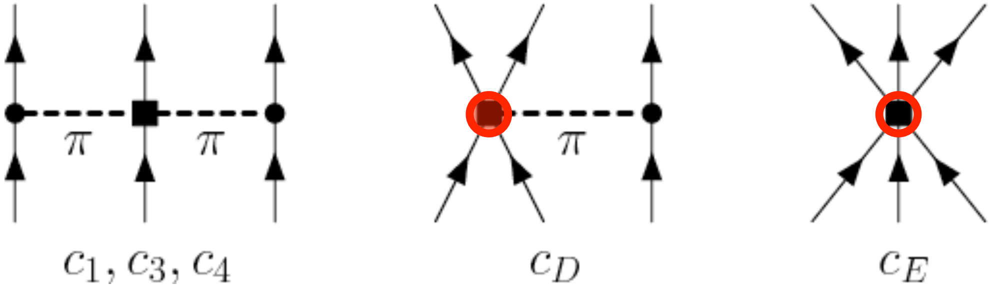
Universal at low-momentum

$V_{\mathrm{low}\,k}(\Lambda)$: lower cutoffs advantageous for nuclear structure calculations

Chiral Effective Field Theory: 3N Forces



Two new couplings at N^{2}LO



c terms given from NN fits: constrained by NN, πN data

c_D c_E fit to properties of light nuclei: Triton binding energy, ^{4}He radius

Strategy

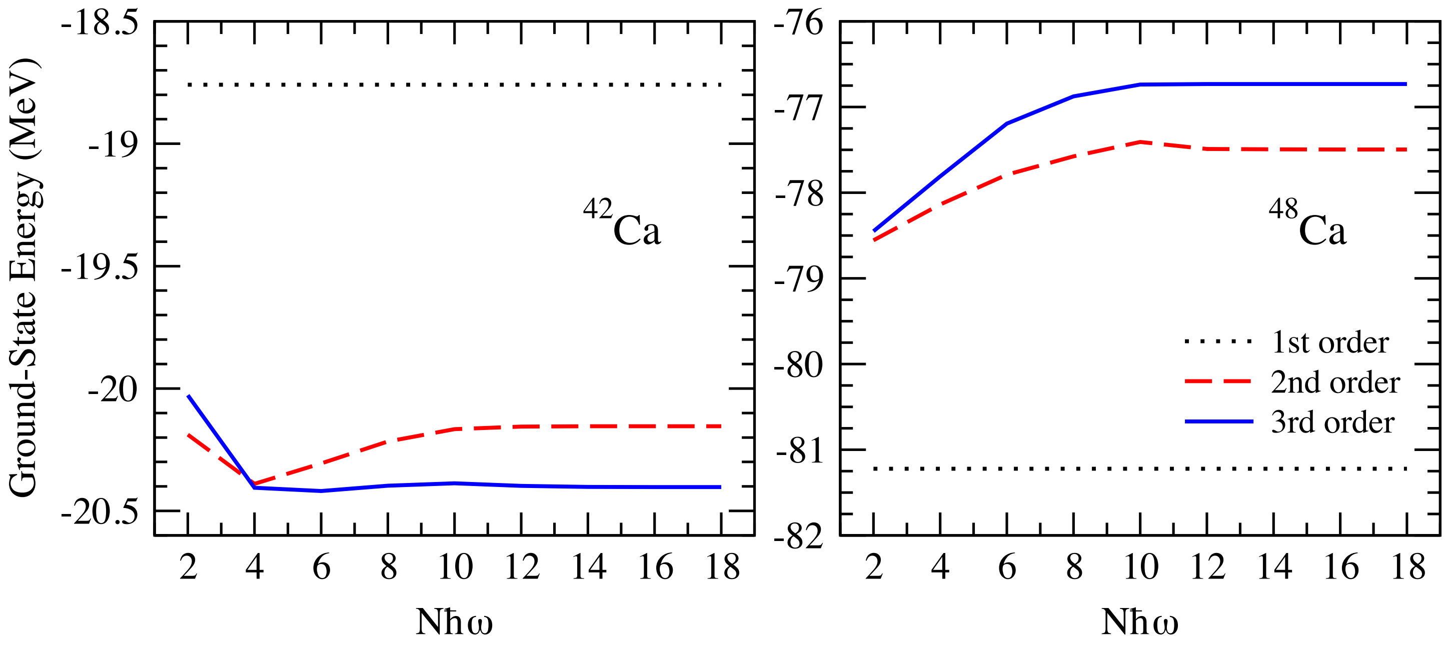
1) Effective interaction: sum excitations outside valence space to **3^{rd} order**

2) Single-particle energies calculated self-consistently

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

4) NN and 3N forces – fully to 3^{rd}-order MBPT

5) Work in extended valence spaces



Clear convergence with HO basis size

Promising order-by-order behavior

Strategy

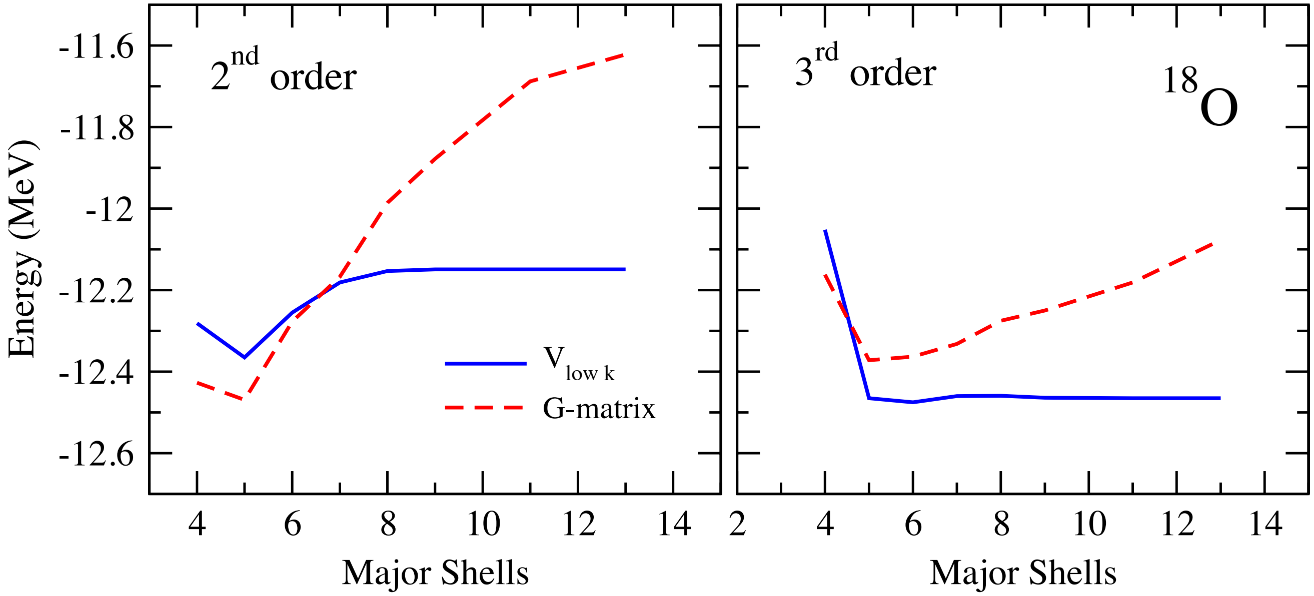
1) Effective interaction: sum excitations outside valence space to **3^{rd} order**

2) Single-particle energies calculated self-consistently

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

4) NN and 3N forces – fully to 3^{rd}-order MBPT

5) Work in extended valence spaces



G-matrix – no signs of convergence (similar in pf-shell)

Strategy

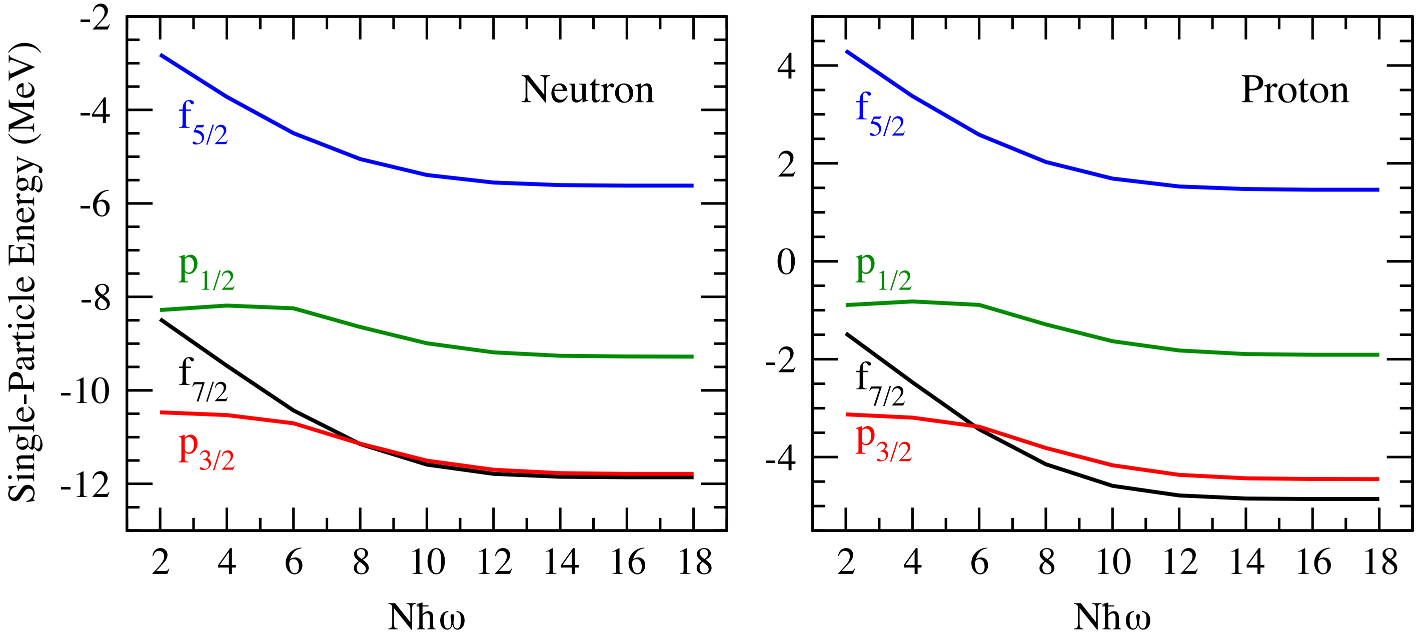
1) Effective interaction: sum excitations outside valence space to **3rd order**

2) Single-particle energies calculated self-consistently

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

4) NN and 3N forces – fully to 3rd-order MBPT

5) Work in extended valence spaces



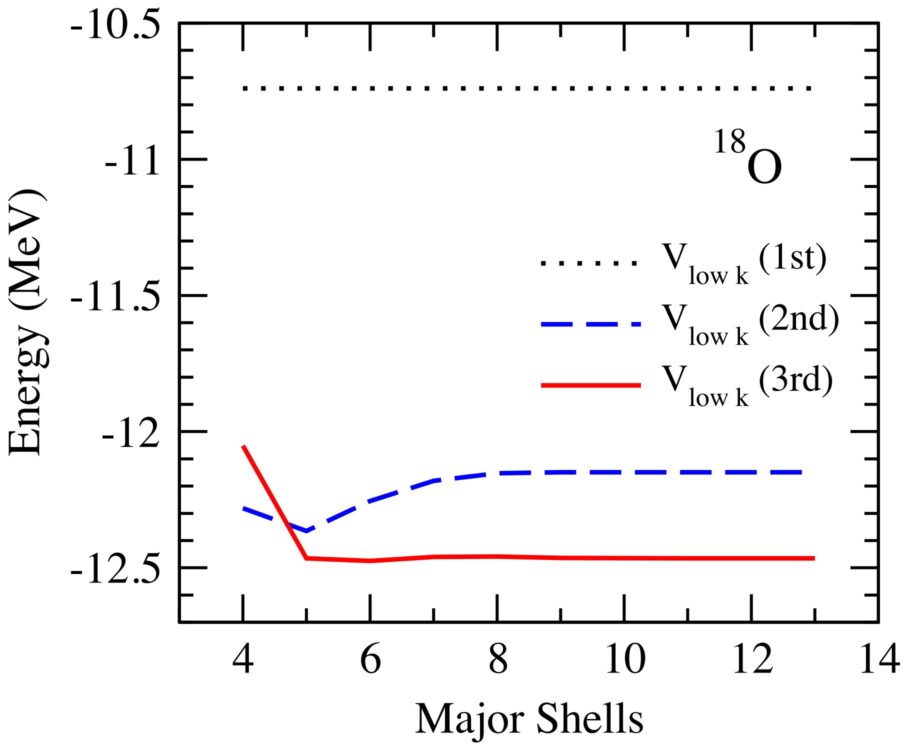
Clear convergence with HO basis size

Promising order-by-order behavior

Convergence Properties

NN matrix elements derived from:

- Chiral N^3LO (Machleidt, 500 MeV) using smooth-regulator $V_{\text{low }k}$
- Third order in MBPT
- 13 major HO shells for intermediate state configurations



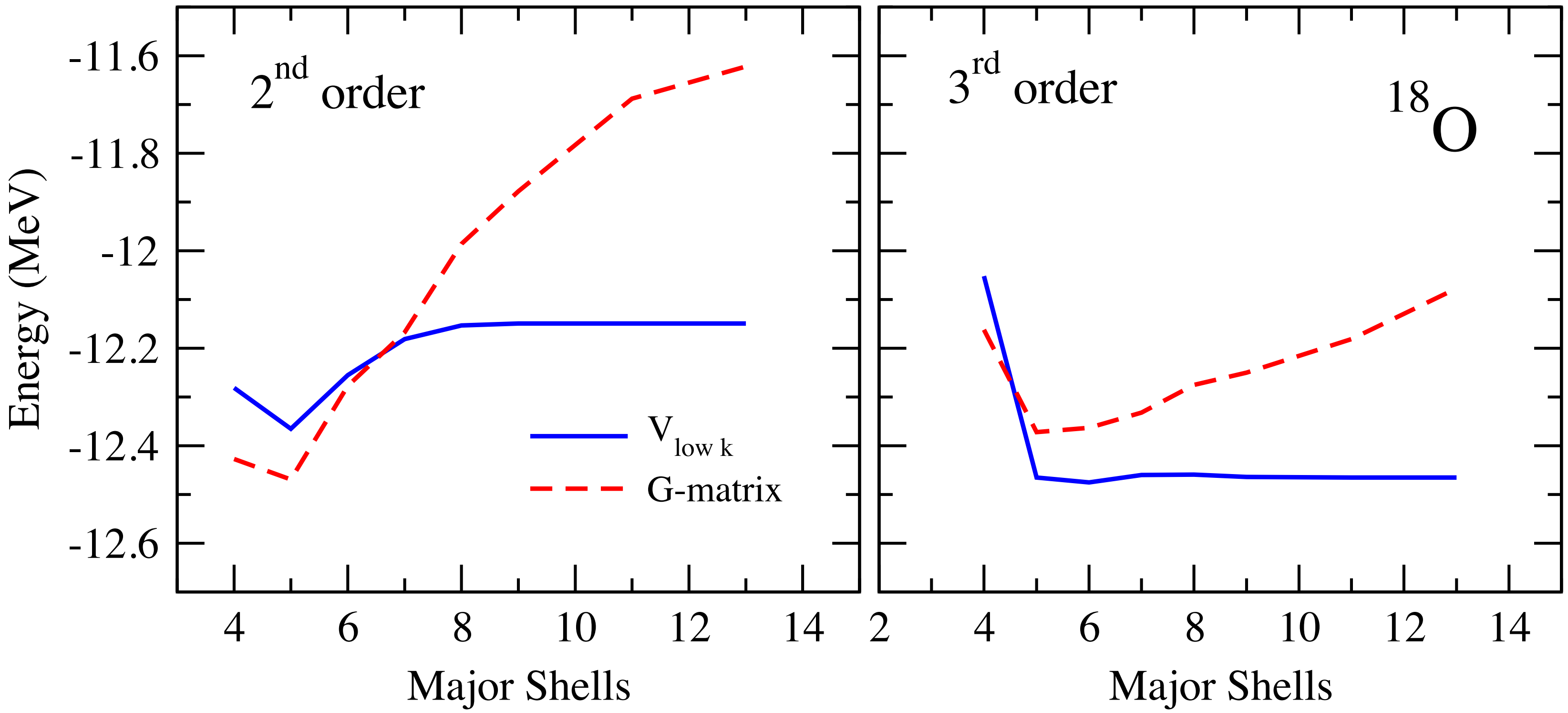
Clear convergence with HO basis size

Promising order-by-order behavior

Convergence Properties

NN matrix elements derived from:

- Chiral N^{3}LO (Machleidt, 500 MeV) using smooth-regulator $V_{\text{low }k}$
- Third order in MBPT
- 13 major HO shells for intermediate state configurations



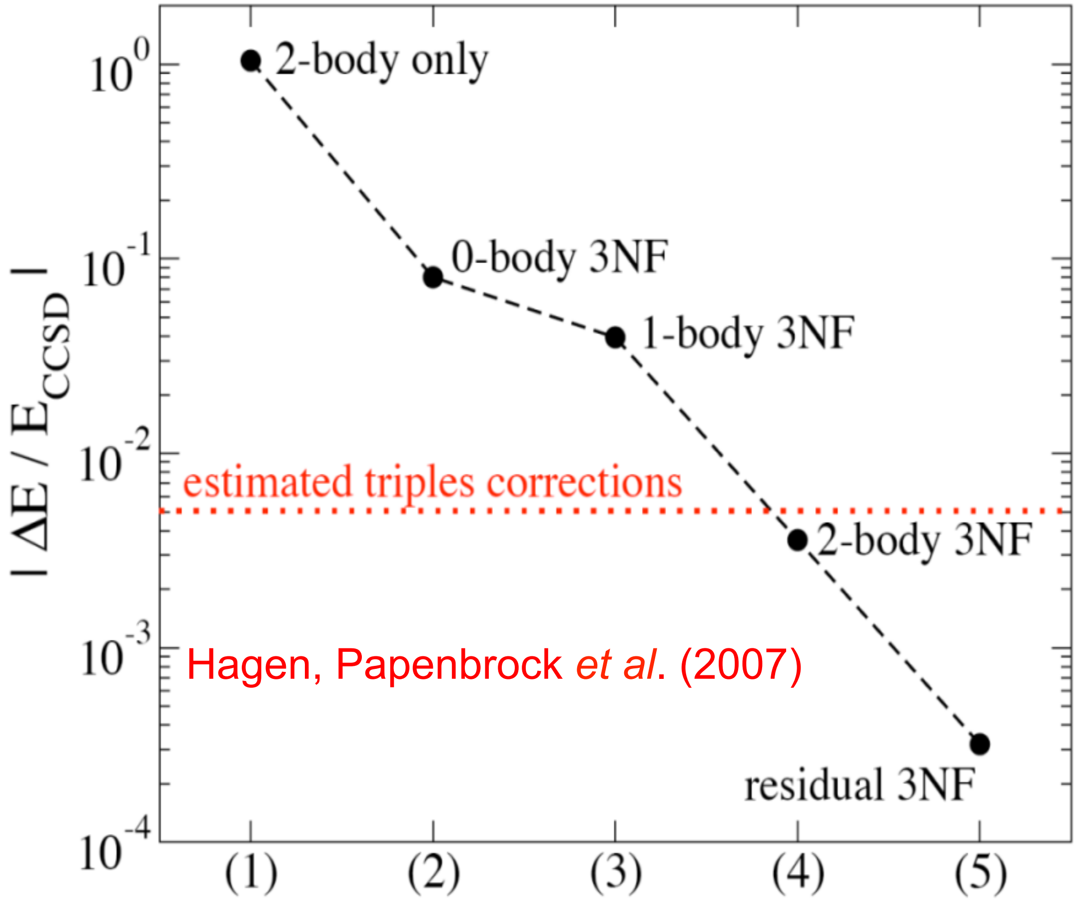
G-matrix – no sign of convergence

3N Forces for Valence-Shell Theories

Effects of residual 3N between 3 valence nucleons?

Normal-ordered 3N: microscopic contributions to inputs for CI Hamiltonian

Effects of residual 3N between 3 valence nucleons?



Hagen, Papenbrock *et al*. (2007)

Coupled-Cluster theory with 3N:
benchmark of ^{4}He

0- 1- and 2-body of 3NF dominate

Residual 3N can be neglected

Work on ^{16}O in progress

Approximated residual 3N by summing over valence nucleon

– Nucleus-dependent: effect small, not negligible by ^{24}O

Backup Intro

From QCD to Nuclear Interactions

How do we determine interactions between nucleons?

$$\boxed{H(\Lambda) = T + V_{\mathrm{NN}}(\Lambda) + V_{\mathrm{3N}}(\Lambda) + V_{\mathrm{4N}}(\Lambda) + \ldots}$$

The image cannot be displayed. Your computer may not have enough memory to open the image, or the image may have been corrupted. Restart your computer, and then open the file again. If the red x still appears, you may have to delete the image and then insert it again.

Effective Hamiltonian – resolution dependent

Only degrees of freedom relevant to energy scale

The image cannot be displayed. Your computer may not have enough memory to open the image, or the image may have been corrupted. Restart your computer, and then open the file again. If the red x still appears, you may have to delete the image and then insert it again.

Increased Resolution

$\Lambda_{\mathrm{chiral}} \sim 700\mathrm{MeV}$

Appropriate separation of scales

Typical momenta in nucleus Q~ $\mathbf{m}_{\pi}$

Effective theory: only nucleons and pions

Monopole Part of Valence-Space Interactions

Microscopic MBPT – effective interaction in chosen model space

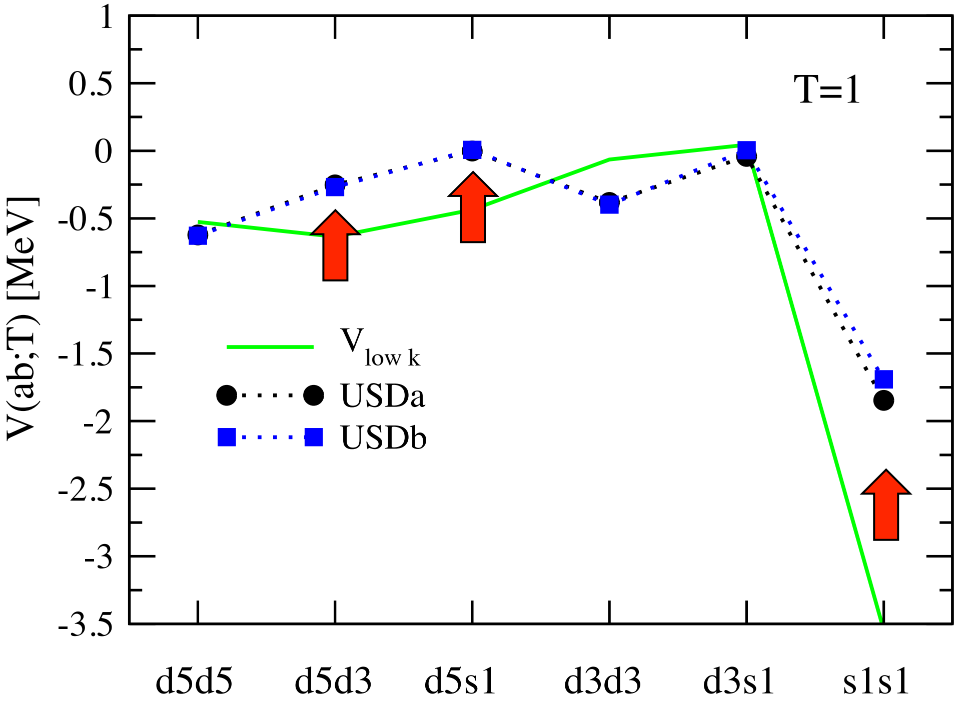
Works near closed shells: deteriorates beyond this

Deficiencies improved adjusting particular two-body matrix elements

Monopoles:
Angular average of interaction

$$V_{ab}^{T} = \frac{\sum_J (2J+1)\ V_{abab}^{JT}}{\sum_J (2J+1)}$$

Determines interaction of orbit *a* with *b*: *evolution of orbital energies*



Microscopic **low-momentum** interactions

Phenomenological **USD** interactions

Clear shifts in **low-lying orbitals**:
- T=1 repulsive shift

Origin of shifts: Neglected 3N forces
-- **Zuker (2003)**

Drip Lines and Magic Numbers: The Nuclear Landscape Toward the Extremes

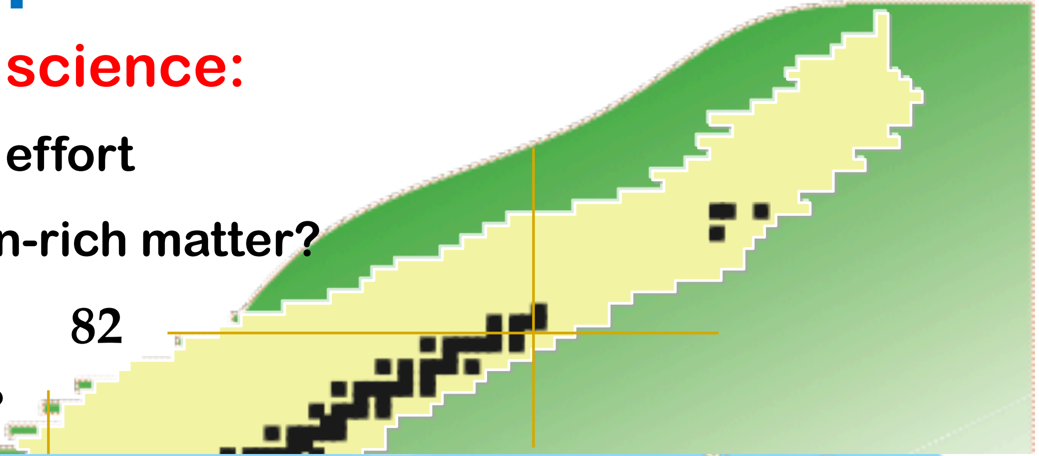
Exploring the frontiers of nuclear science:

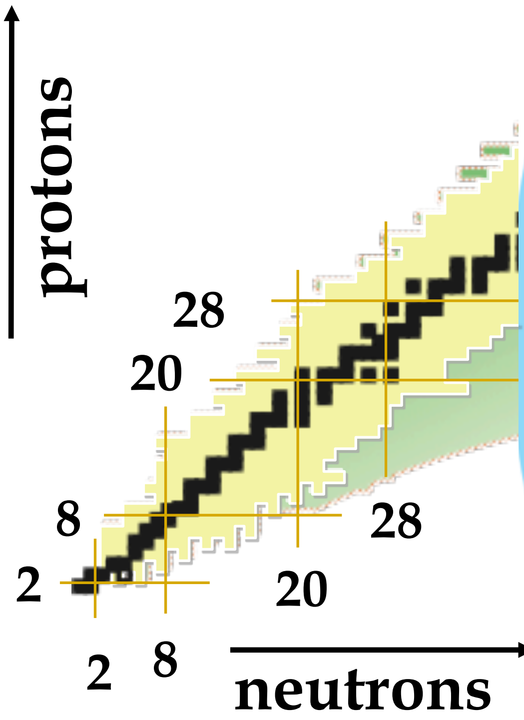
Worldwide joint **experimental**/theoretical effort

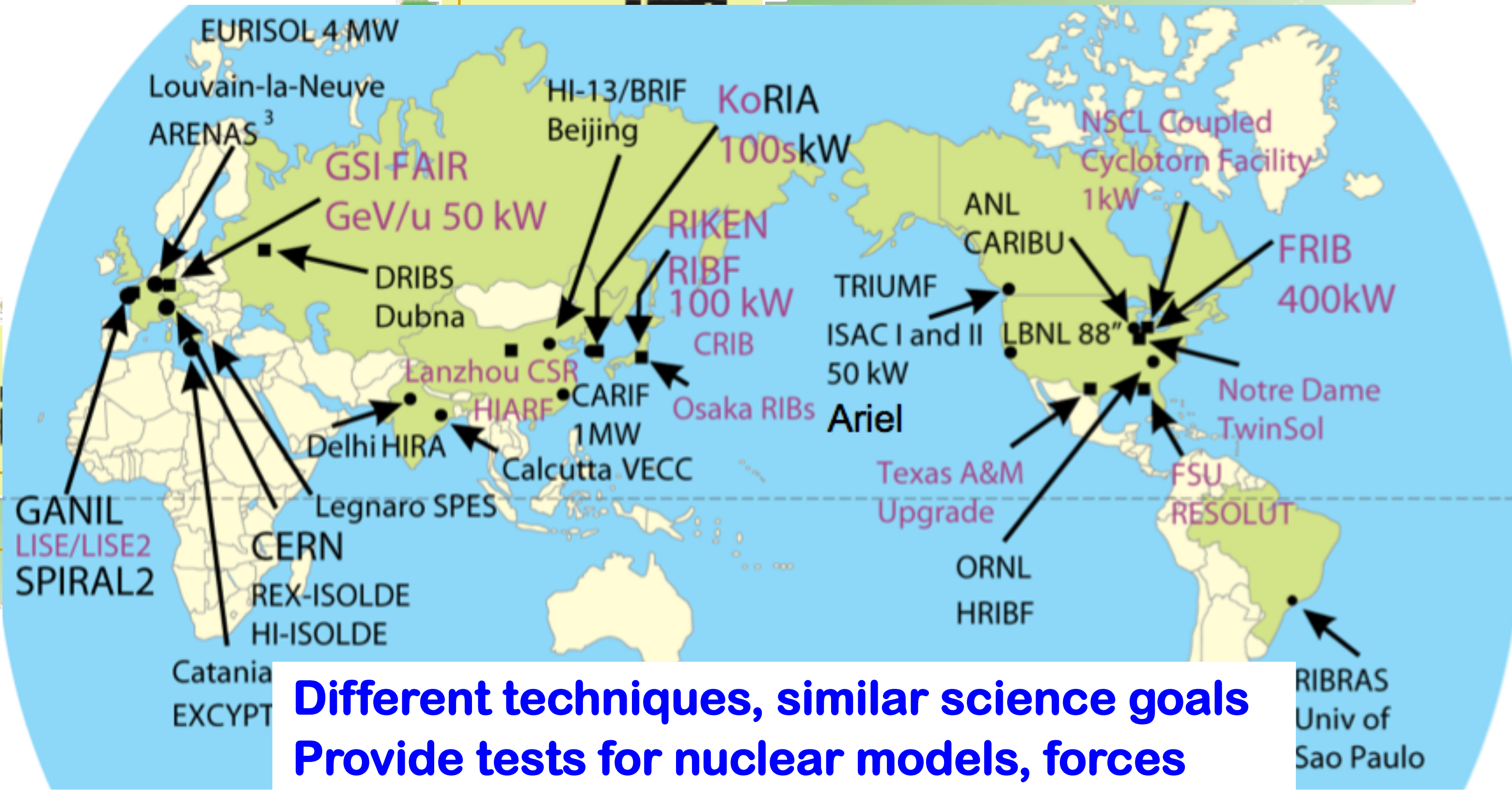
What are the properties of proton/neutron-rich matter?

What are the limits of nuclear existence?

How do magic numbers form and evolve?







Different techniques, similar science goals
Provide tests for nuclear models, forces

Theory: points to key measurements

Perturbative Valence-Space Strategy

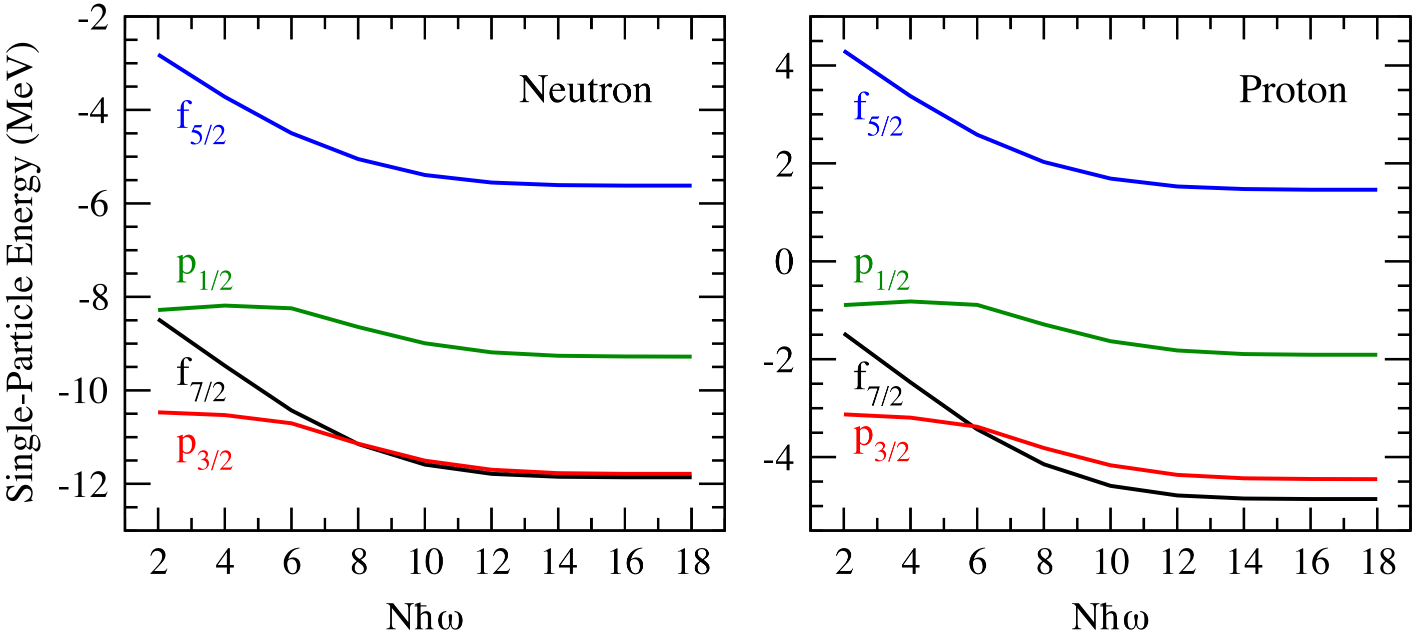
1) Effective interaction: sum excitations outside valence space to **3^{rd} order**

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

5) Explore extended valence spaces



Clear convergence with HO basis size

Promising order-by-order behavior

Drip Lines and Magic Numbers: The Nuclear Landscape Toward the Extremes

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?