Ab Initio Valence-Space Hamiltonians for Exotic Nuclei

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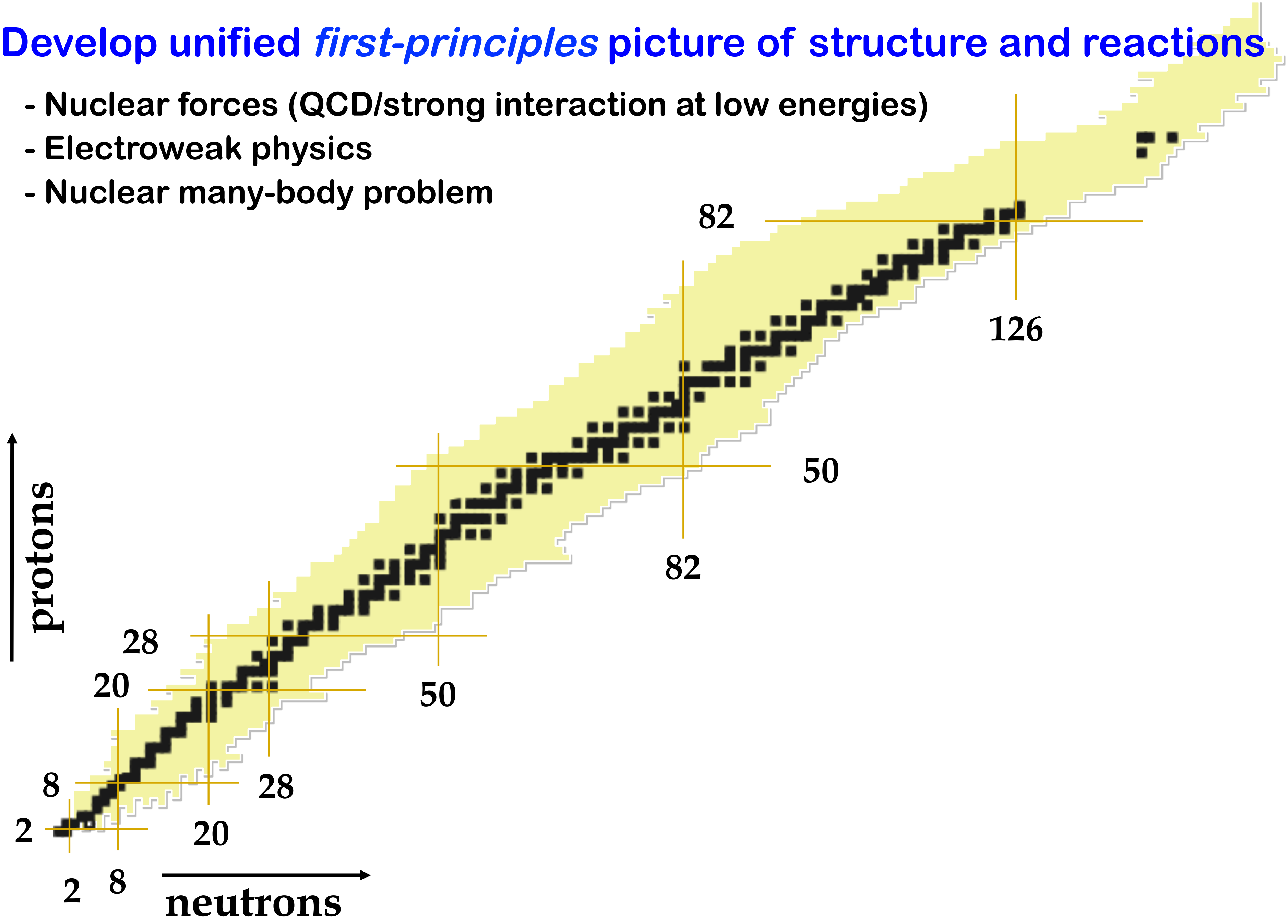
Frontiers and Impact of Nuclear Science

Aim of ab initio nuclear theory:

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

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



Medium- and Heavy-Mass Exotic Nuclei

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

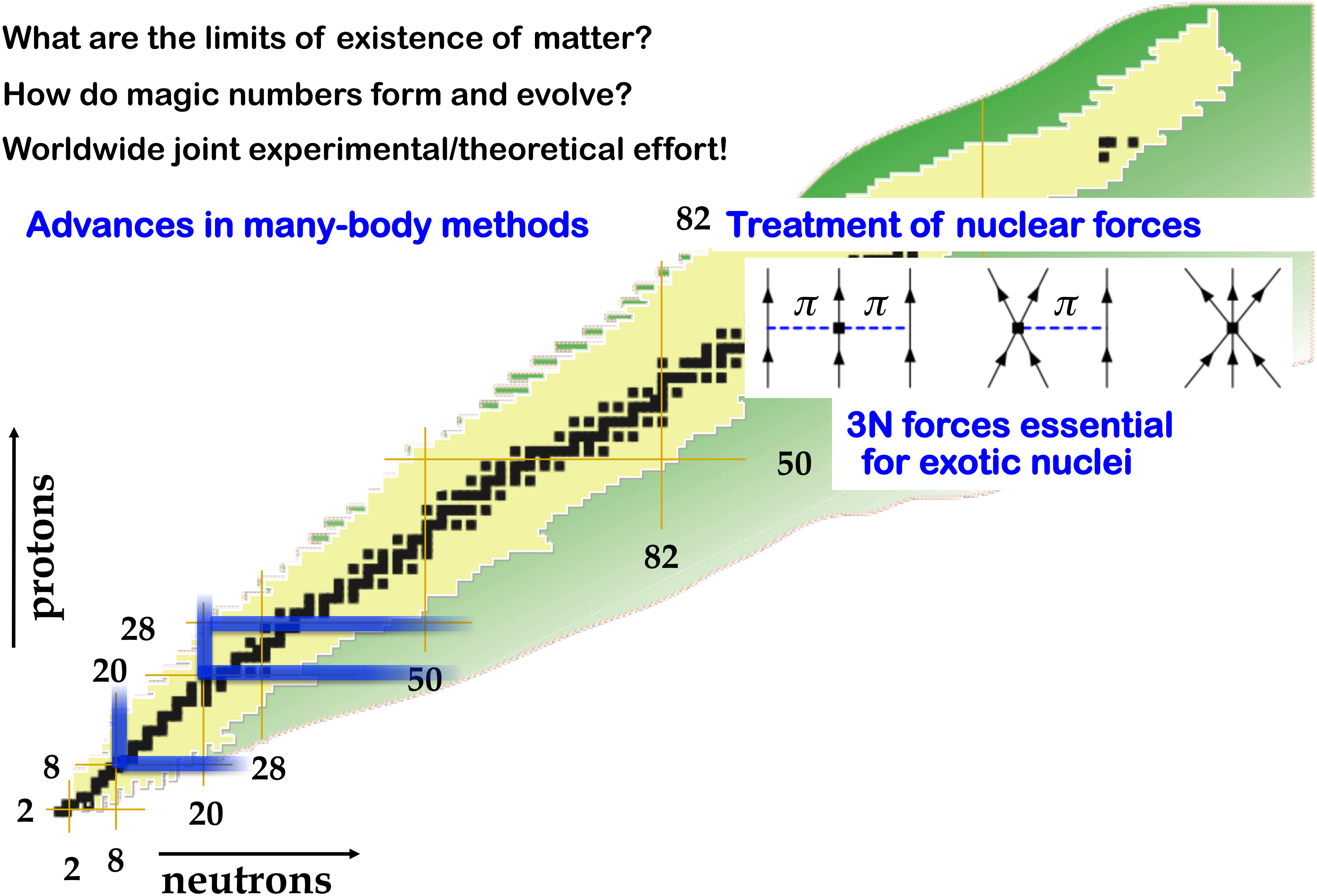
What are the limits of existence of matter?

How do magic numbers form and evolve?

Worldwide joint experimental/theoretical effort!

Advances in many-body methods

Treatment of nuclear forces



3N forces essential for exotic nuclei

The Nuclear Many-Body Problem

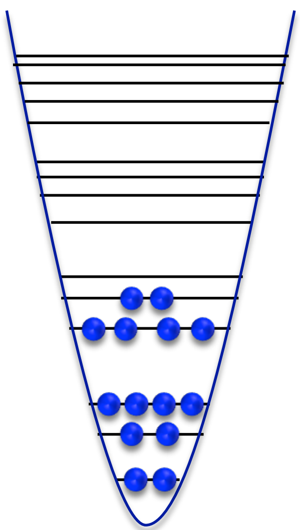
Nucleus strongly interacting many-body system – A-body problem impossible

$$H\psi_n = E_n\psi_n$$

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

Large space: controlled approximations to full Schrödinger Equation

Large-space approach



Limited range:

Closed shell ± 1

Even-even

Limited properties:

Ground states only

Some excited state

Coupled Cluster

In-Medium SRG

Green's Function

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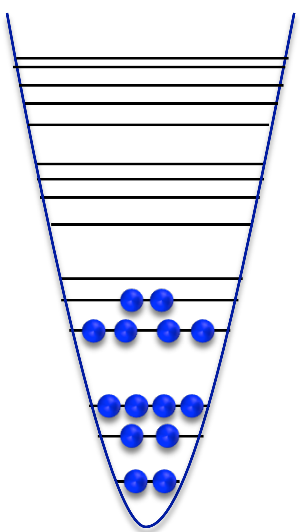
Valence space: diagonalize exactly with reduced number of degrees of freedom

Large-space approach



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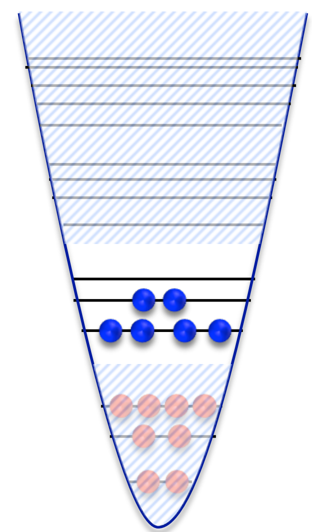

All nuclei near closed-shell cores

All properties:

Ground states

Excited states

EW transitions

Coupled Cluster

In-Medium SRG

Perturbation Theory

In-Medium Similarity Renormalization Group

Continuous unitary trans (basis change) decouples "off-diagonal" physics

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

Interaction in new basis is simple

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

In-Medium SRG

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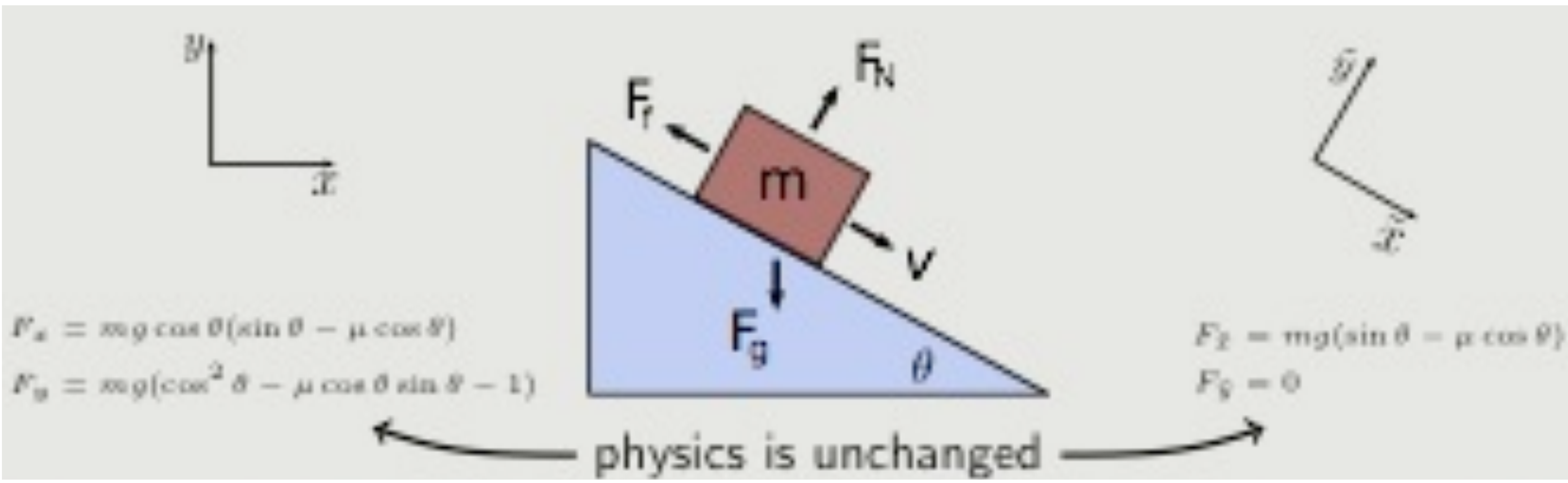


Can always write $U = e^{\eta}$, for some generator η

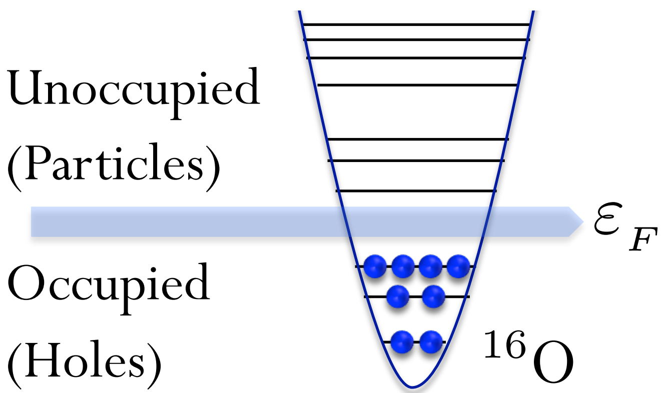
For incline plane: $\eta = \begin{pmatrix} 0 & \theta \\ -\theta & 0 \end{pmatrix}$

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

Life Is Difficult: Particle/Hole Excitations

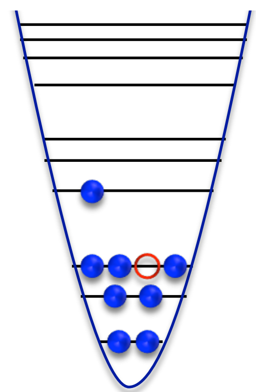
Consider basis states as excitations from uncorrelated reference state

Ref. Slater Determinant



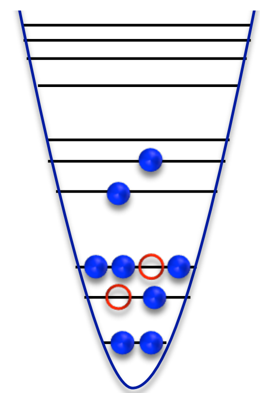
$$|\Phi_0\rangle = \prod_{i=1}^{N} a_i^\dagger |0\rangle$$

1p-1h excitation



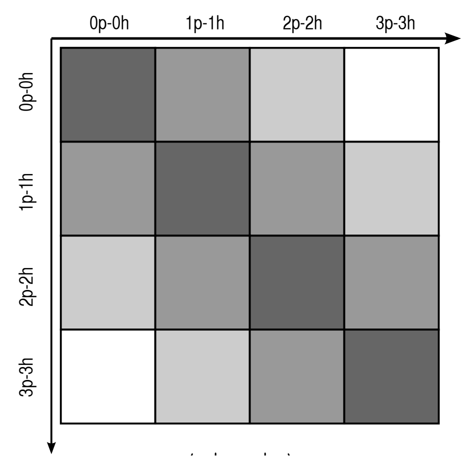
$$|\Phi_i^a\rangle = a_a^\dagger a_i |\Phi_0\rangle$$

2p-2h excitation



$$|\Phi_{ij}^{ab}\rangle = a_a^\dagger a_i a_b^\dagger a_j |\Phi_0\rangle$$

Hamiltonian schematically in terms of ph excitations



$\langle i|H|j\rangle$

Ground-state coupled to excitations is difficult

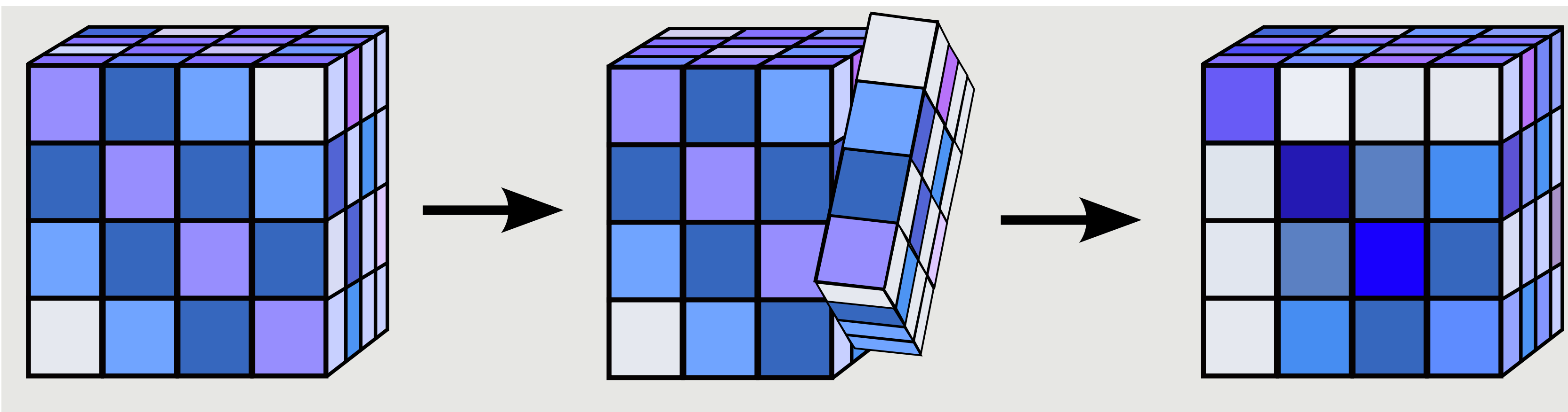
$$H^{\text{od}} = \langle p|H|h\rangle + \langle pp|H|hh\rangle + \cdots + \text{h.c.}$$

In-Medium SRG for Nuclei

For nuclear Hamiltonian, take

$$U = e^{\eta} \text{ with } \eta = \frac{H_{\rm od}}{\Delta} + \text{h.c.}$$

Perform multiple rotations $U_N = e^{\eta_N} \cdots e^{\eta_2} e^{\eta_1}$ until $\eta_N = 0$



$\langle i|H|j\rangle$ $\langle \text{np}n h|\tilde{H}|\Phi_0\rangle = 0$

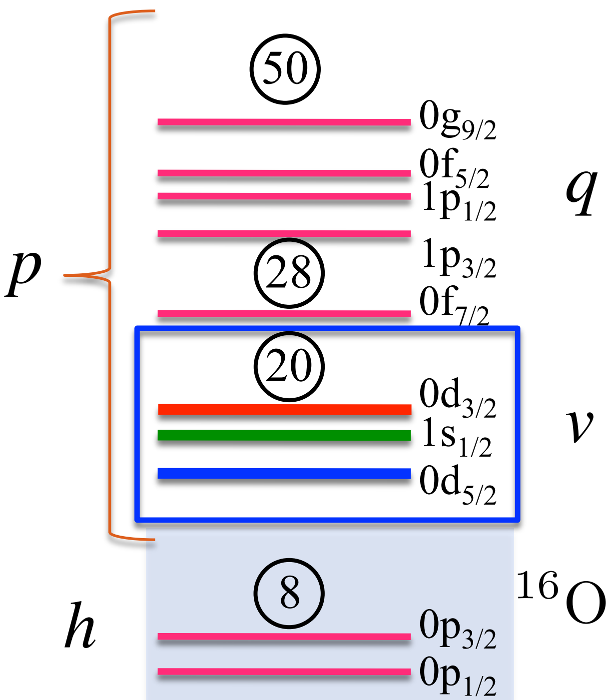
Fully correlated ground state: one matrix element $\langle \Phi_0|\tilde{H}|\Phi_0\rangle$

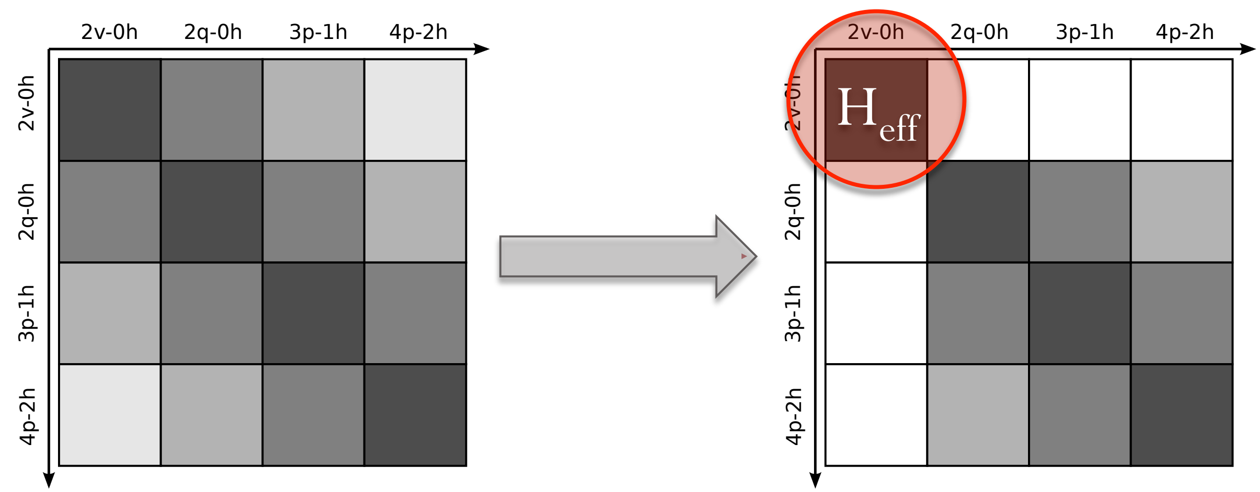
Also flow equation approach $$\frac{\mathrm{d}H(s)}{\mathrm{d}s} = [\eta(s), H(s)]$$

IM-SRG for Valence-Space Hamiltonians

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

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





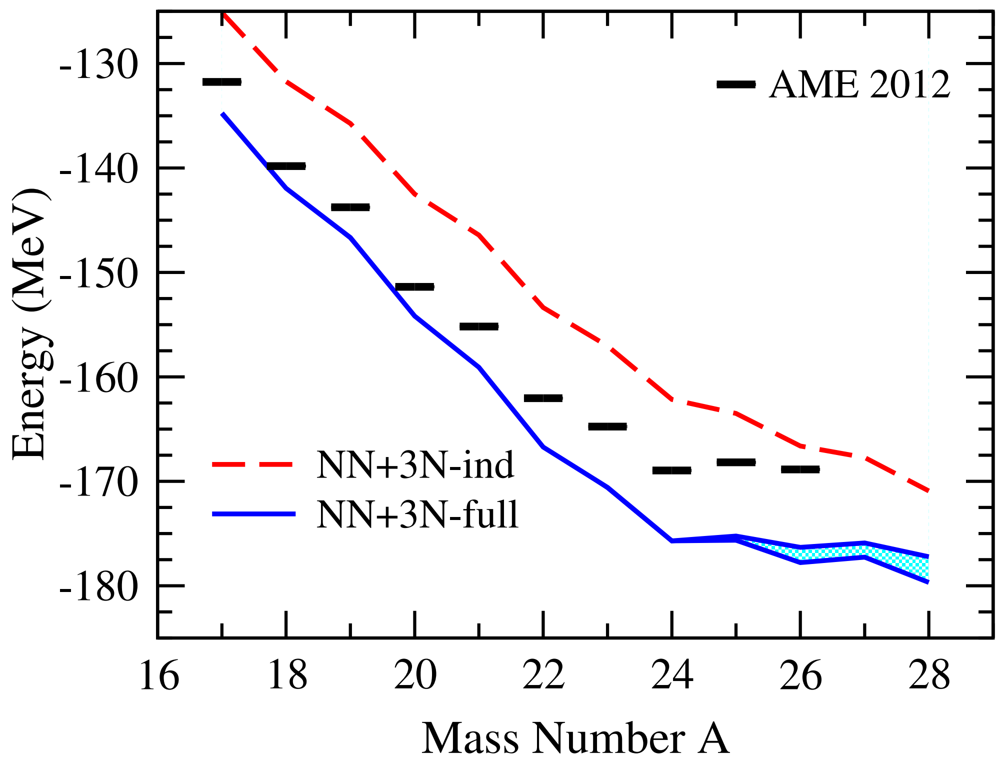
$$H(s=0) \rightarrow H(\infty)$$

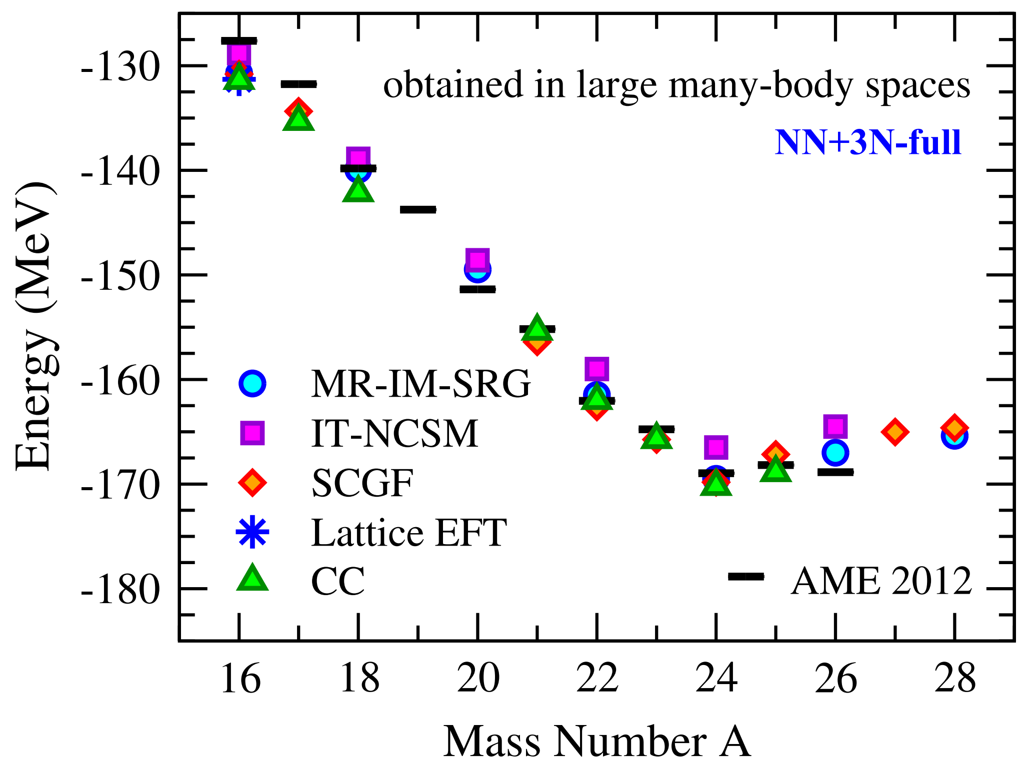
Redefine H^{od} to **decouple valence space from excitations** outside v

$$H^{\mathrm{od}} = \underbrace{\langle p|H|h\rangle + \langle pp|H|hh\rangle}_{\text{Core Energy}} + \underbrace{\langle v|H|q\rangle}_{\text{Single-particle energies}} + \underbrace{\langle pq|H|vv\rangle + \langle pp|H|hv\rangle}_{\text{Two-body valence particle interaction matrix elements}} + \mathrm{h.c.}$$

Ground-State Energies in Oxygen Isotopes

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





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

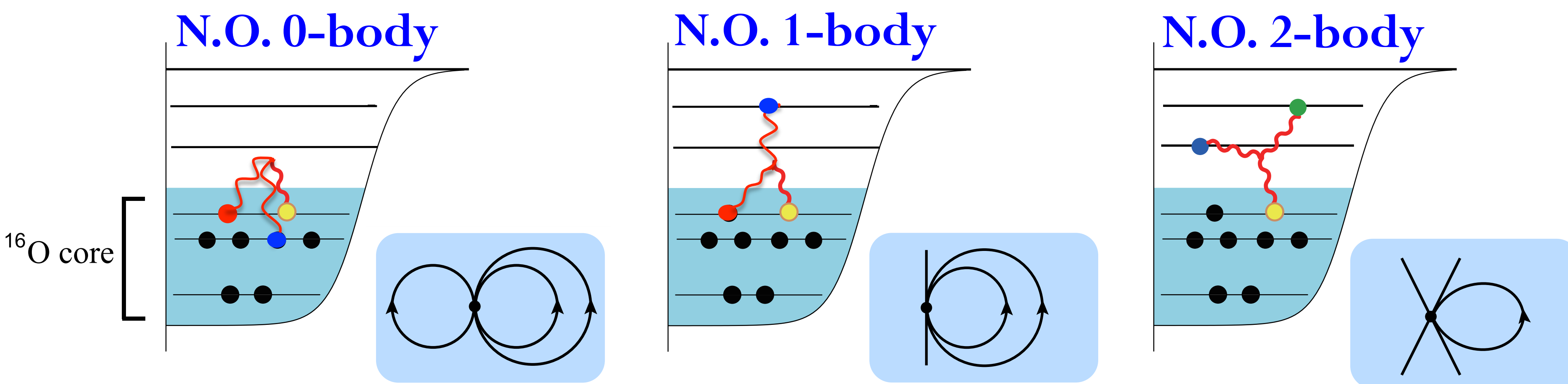
Agreement between all methods with same input forces

Clear improvement with NN+3N-full

Still significant discrepancy between valence/large-space results

How Do We Handle 3N Forces?

Normal-ordered 3N: contribution from core with valence particles

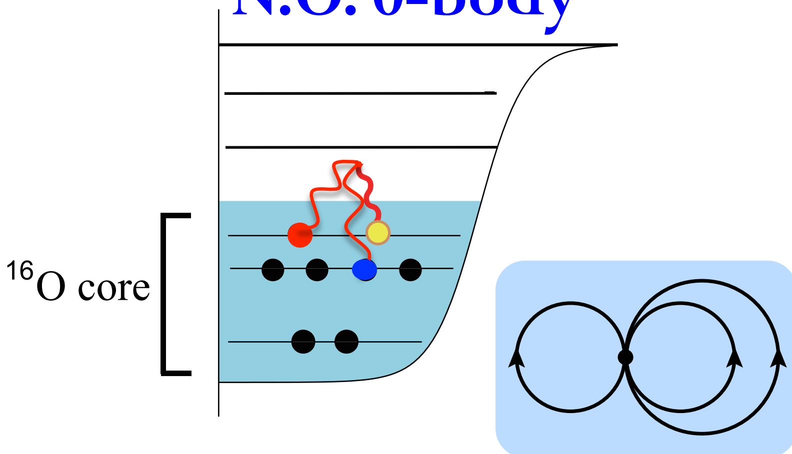


Neglect 3N forces between valence particles – significant as $N_v \sim N_c$

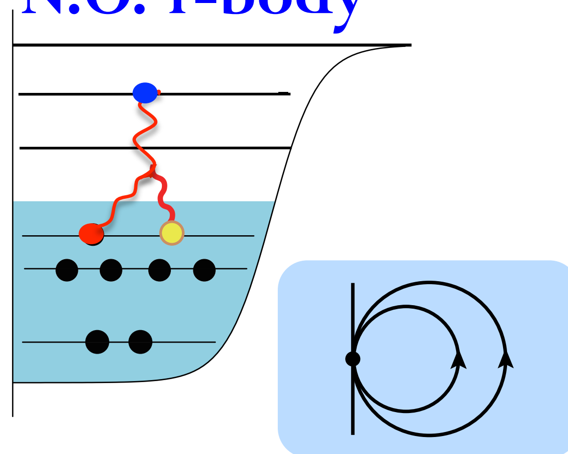
Targeted Normal Ordering

Normal-ordered 3N: contribution from core with valence particles

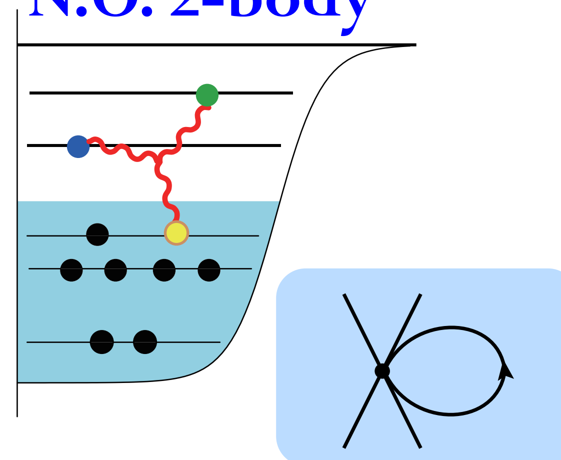
N.O. 0-body



N.O. 1-body



N.O. 2-body



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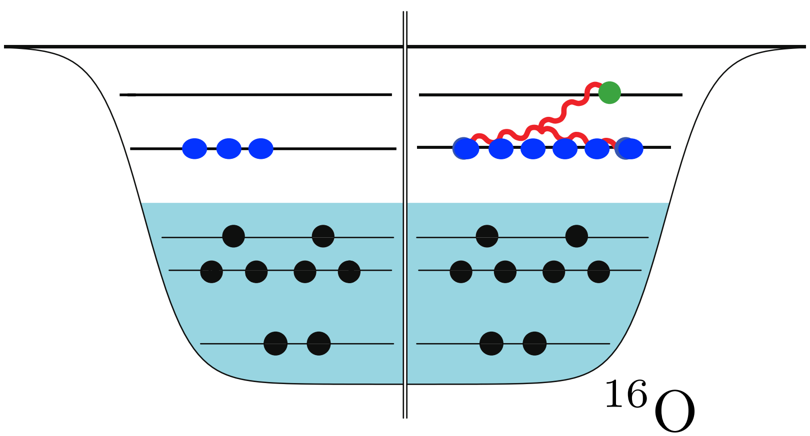
Capture these effects with new **Targeted N.O.**



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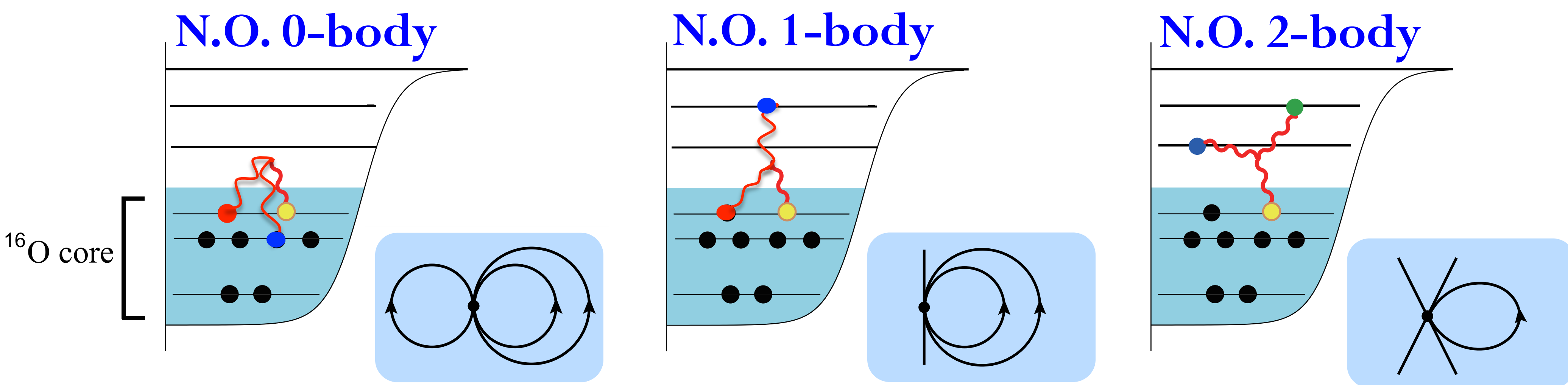

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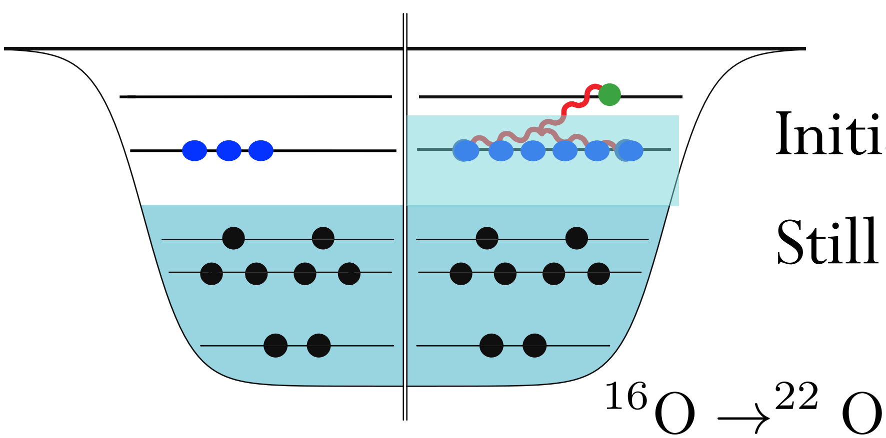
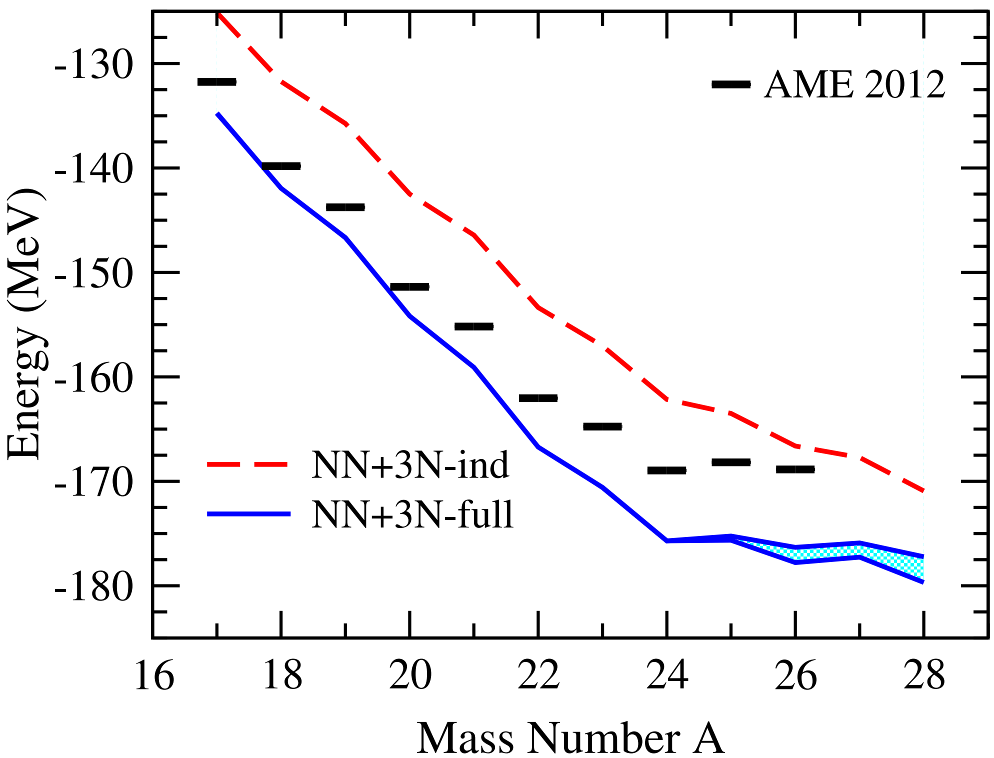


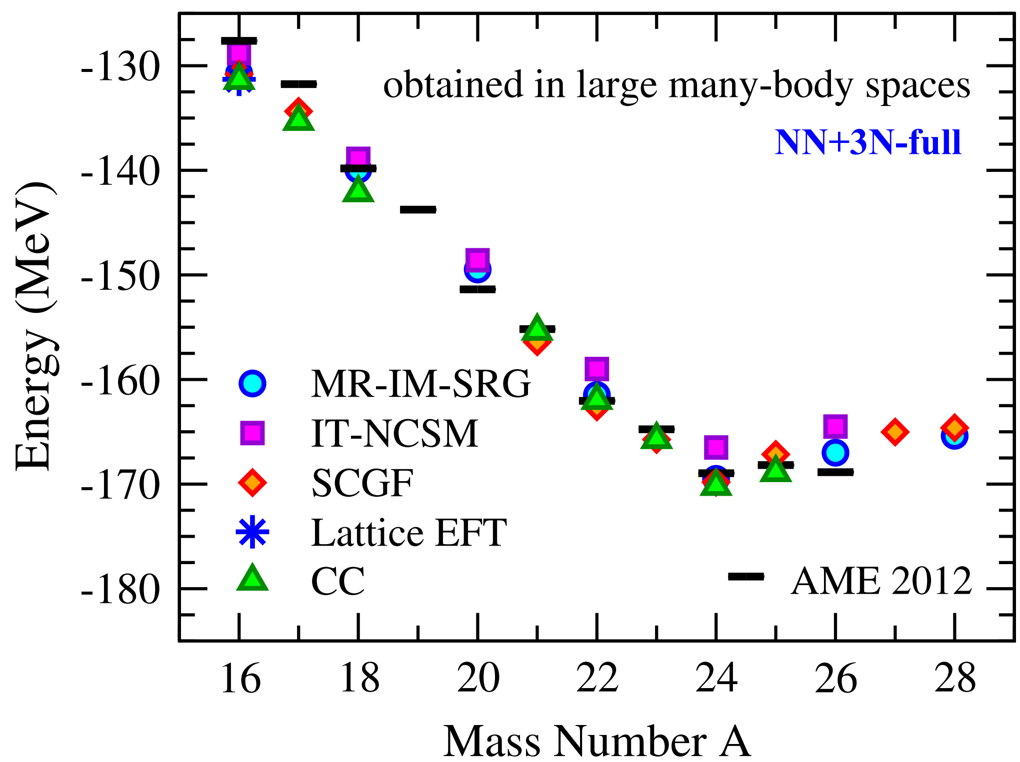
Initial N.O. wrt **nearest closed shell**

Still decouple standard *sd* valence space

Ground-State Energies in Oxygen Isotopes

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





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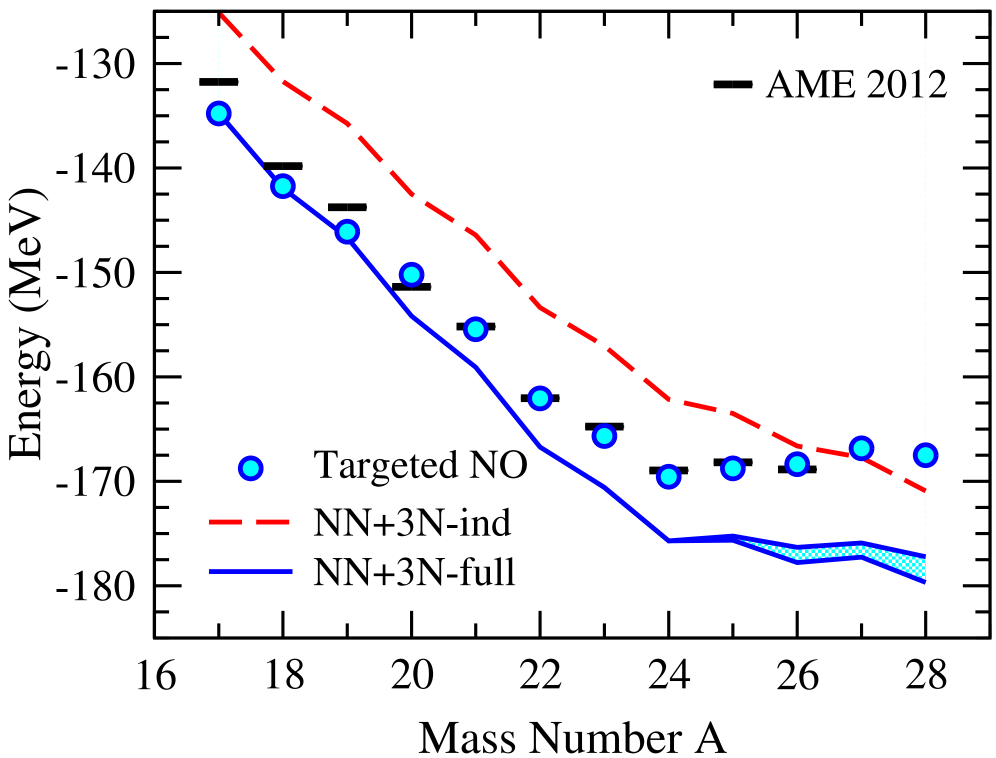
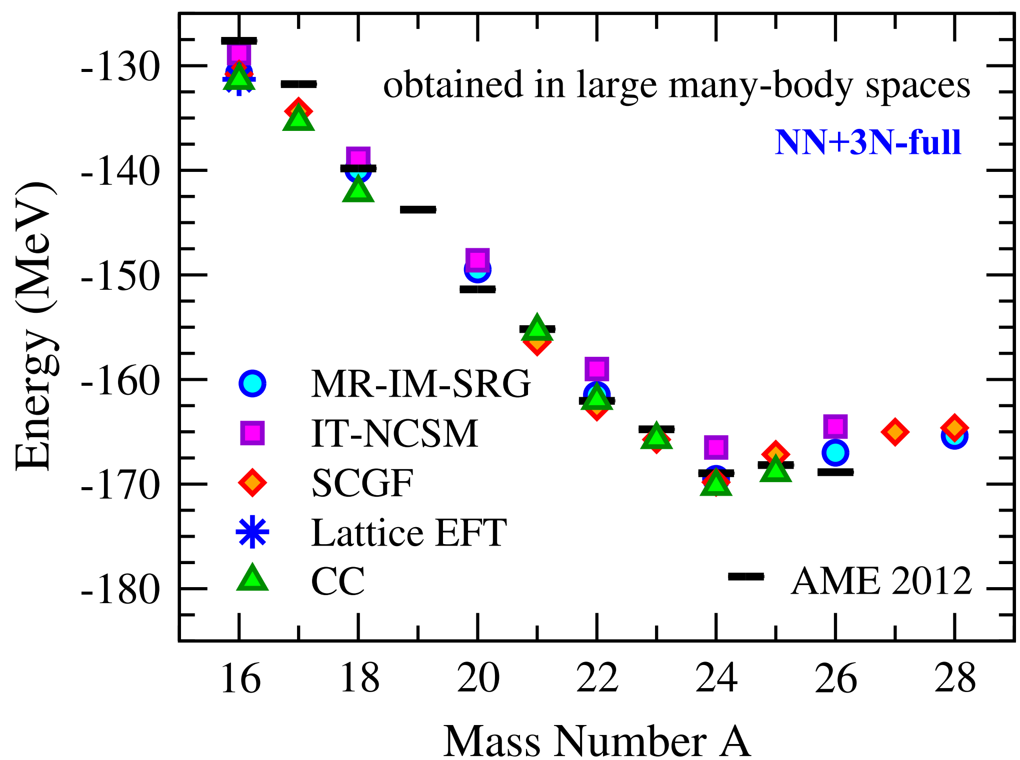




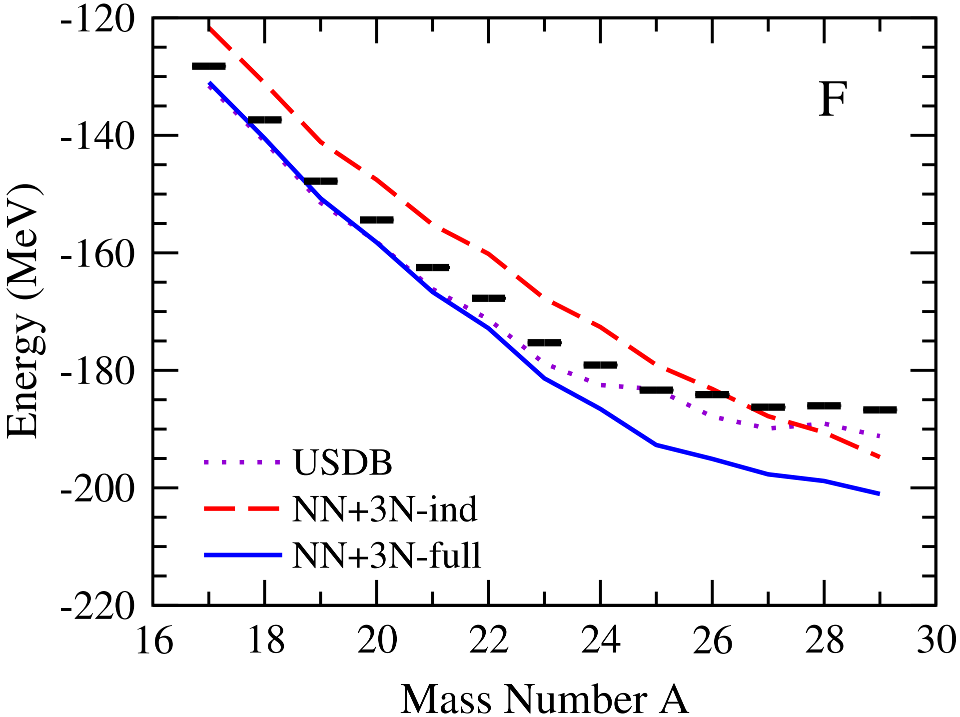
Bogner et al., PRL (2015) Hebeler, JDH, Menéndez, Schwenk, ARNPS (2015)

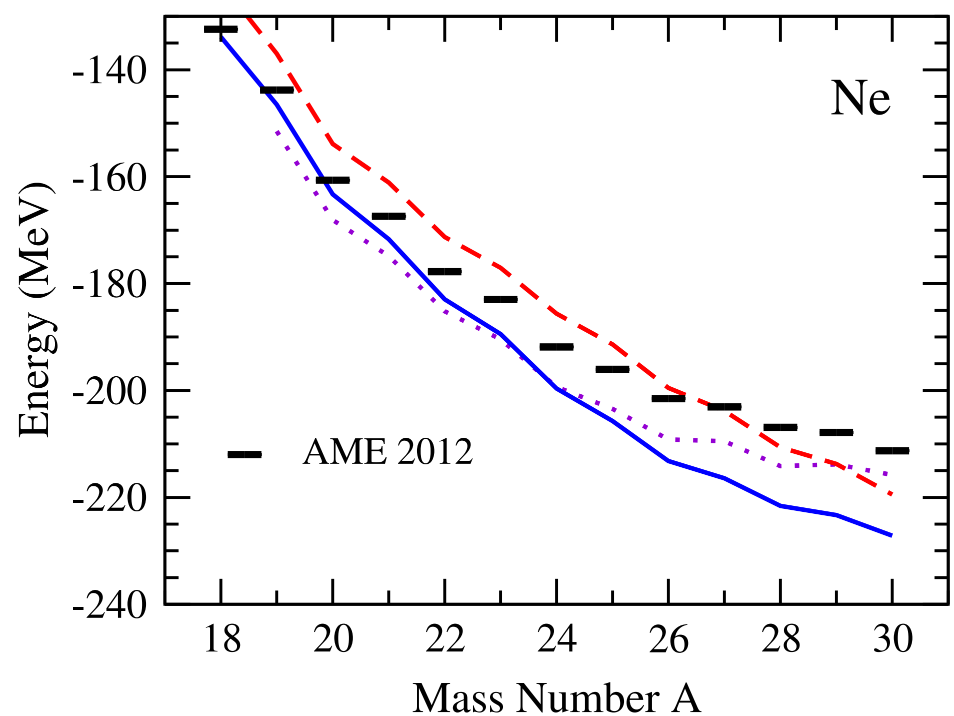
Improved method to capture neglected 3N forces in valence space

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

Beyond Semi-Magic: Ground States of F/Ne

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





Stroberg et al., arXiv:1511.03802

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

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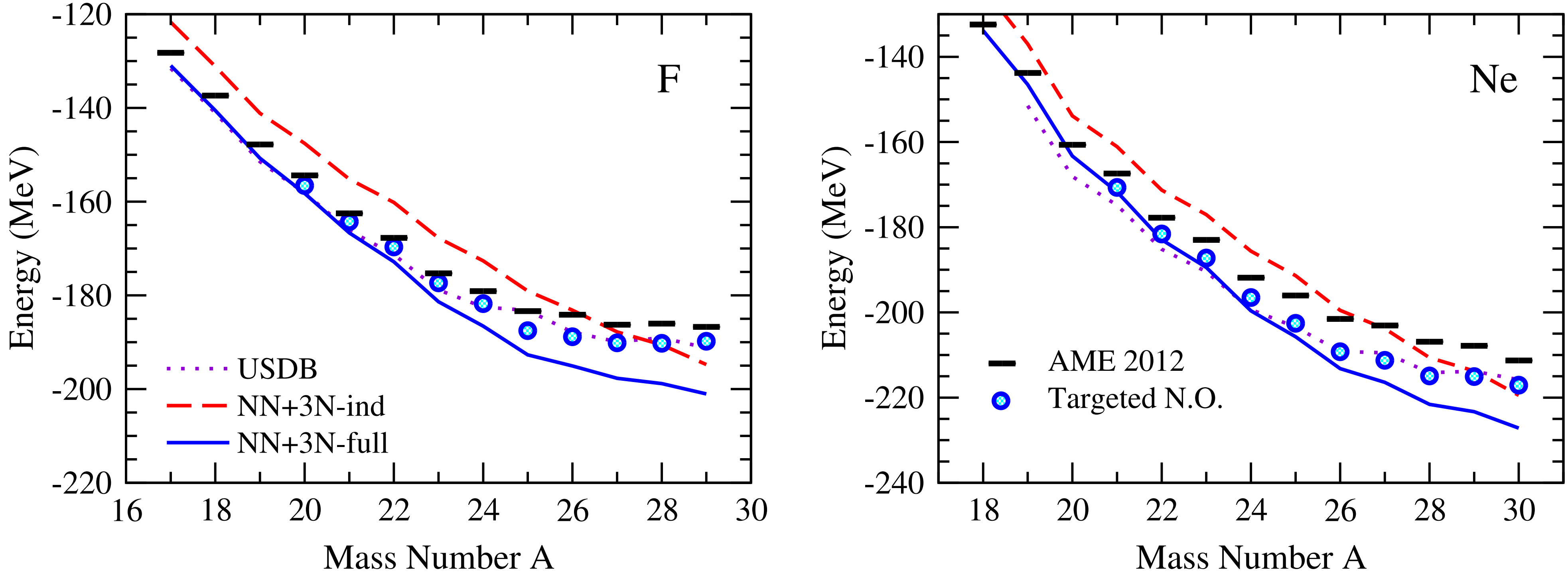

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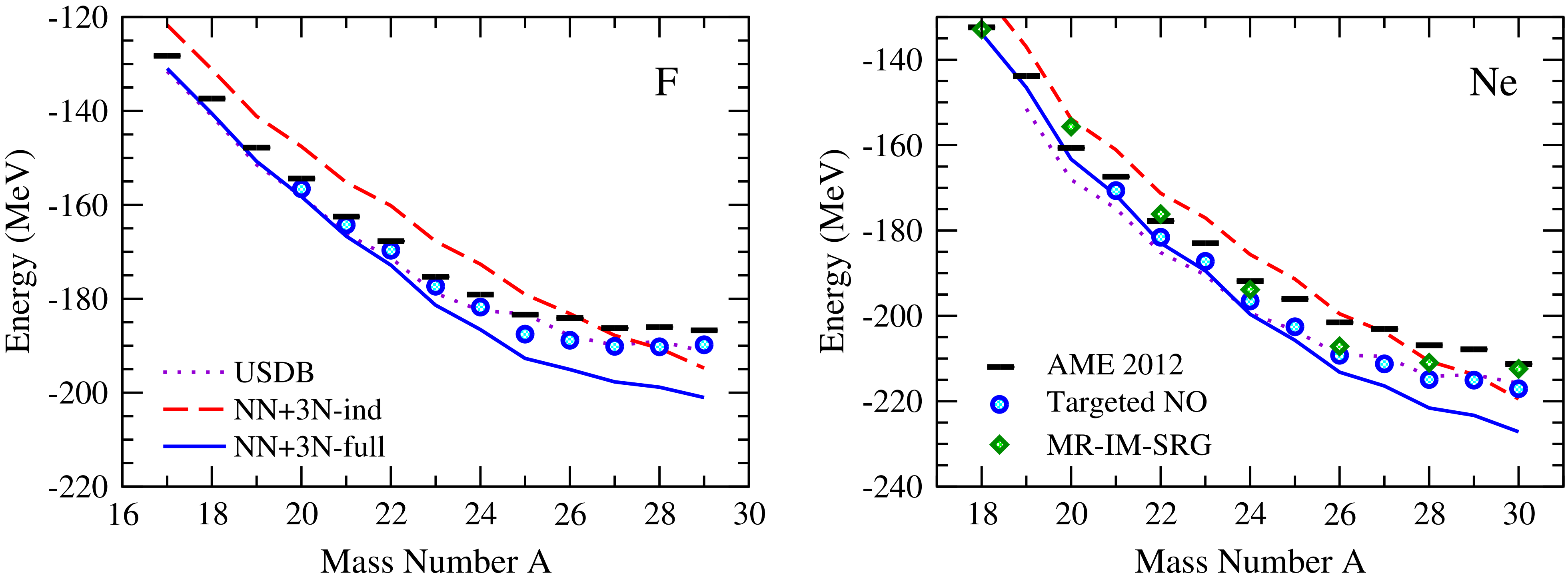

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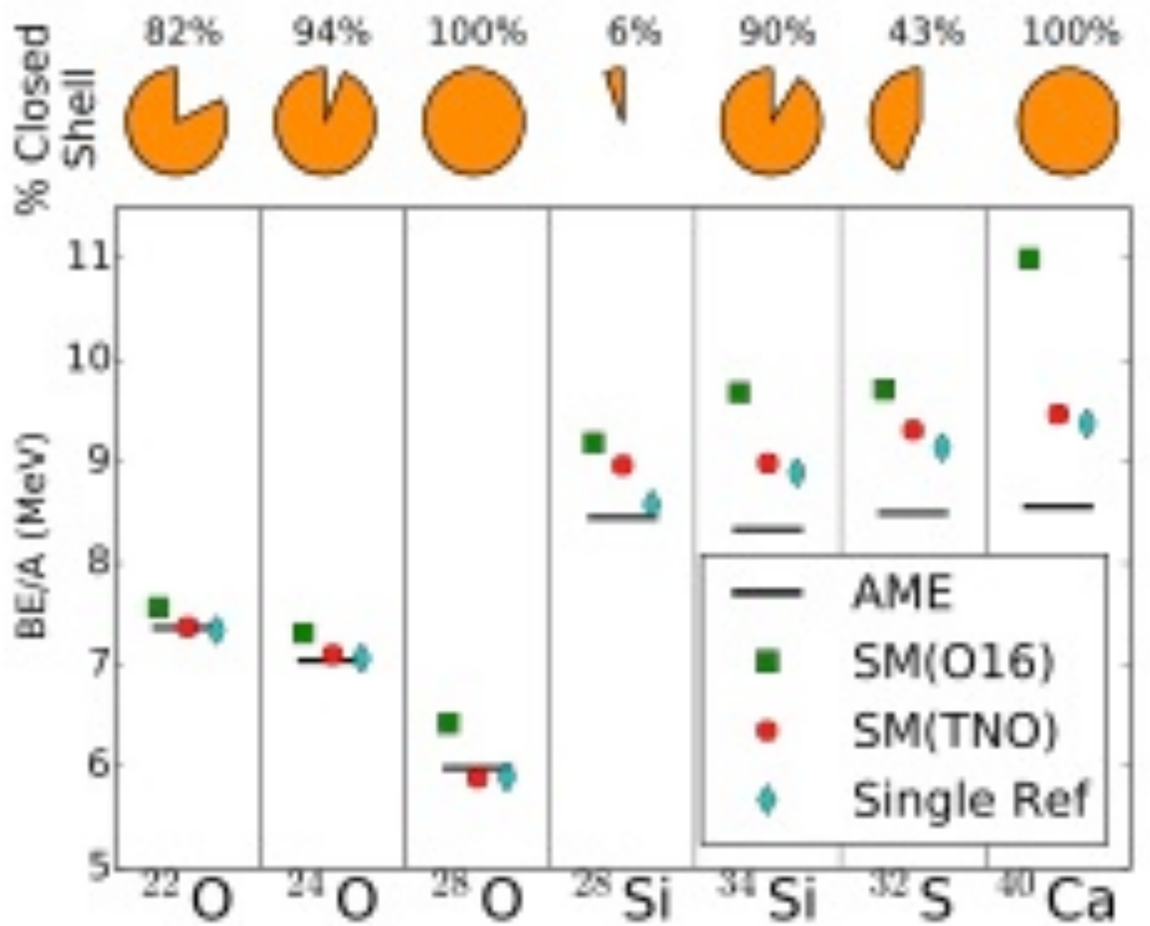
Good agreement with large-space MR-IM-SRG!

Ground States from Oxygen to Calcium

3N force effects significant as N_v becomes large



Stroberg et al., in prep

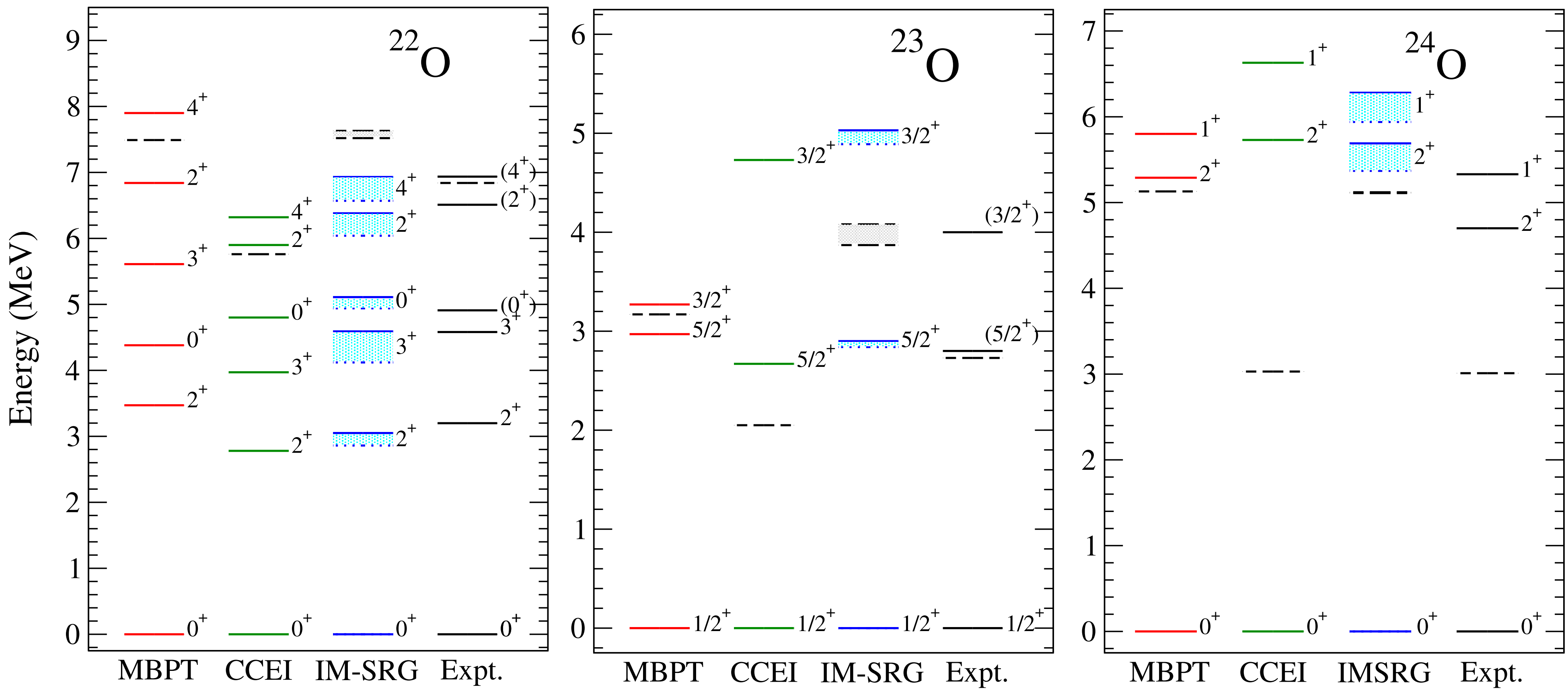
Targeted N.O. valence-space results agrees with large-space in all cases!

^{28}Si not good closed shell (single ref. incorrect)

Discrepancy with experiment from initial nuclear interactions

Comparison with MBPT/CCEI Oxygen Spectra

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



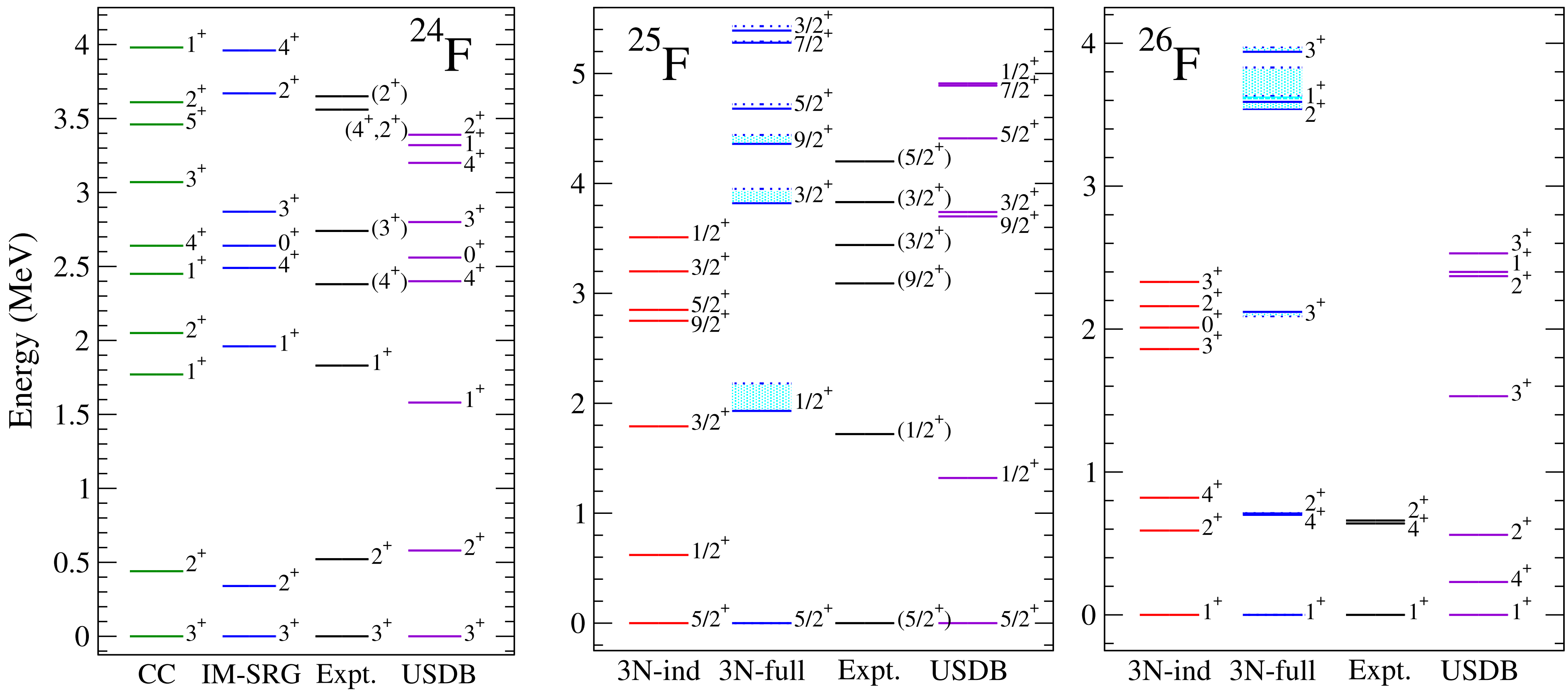
Hebeler, JDH, Menéndez, Schwenk, ARNPS (2015)

MBPT in extended valence space

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

Doubly Open Shell: Neutron-Rich F Spectra

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



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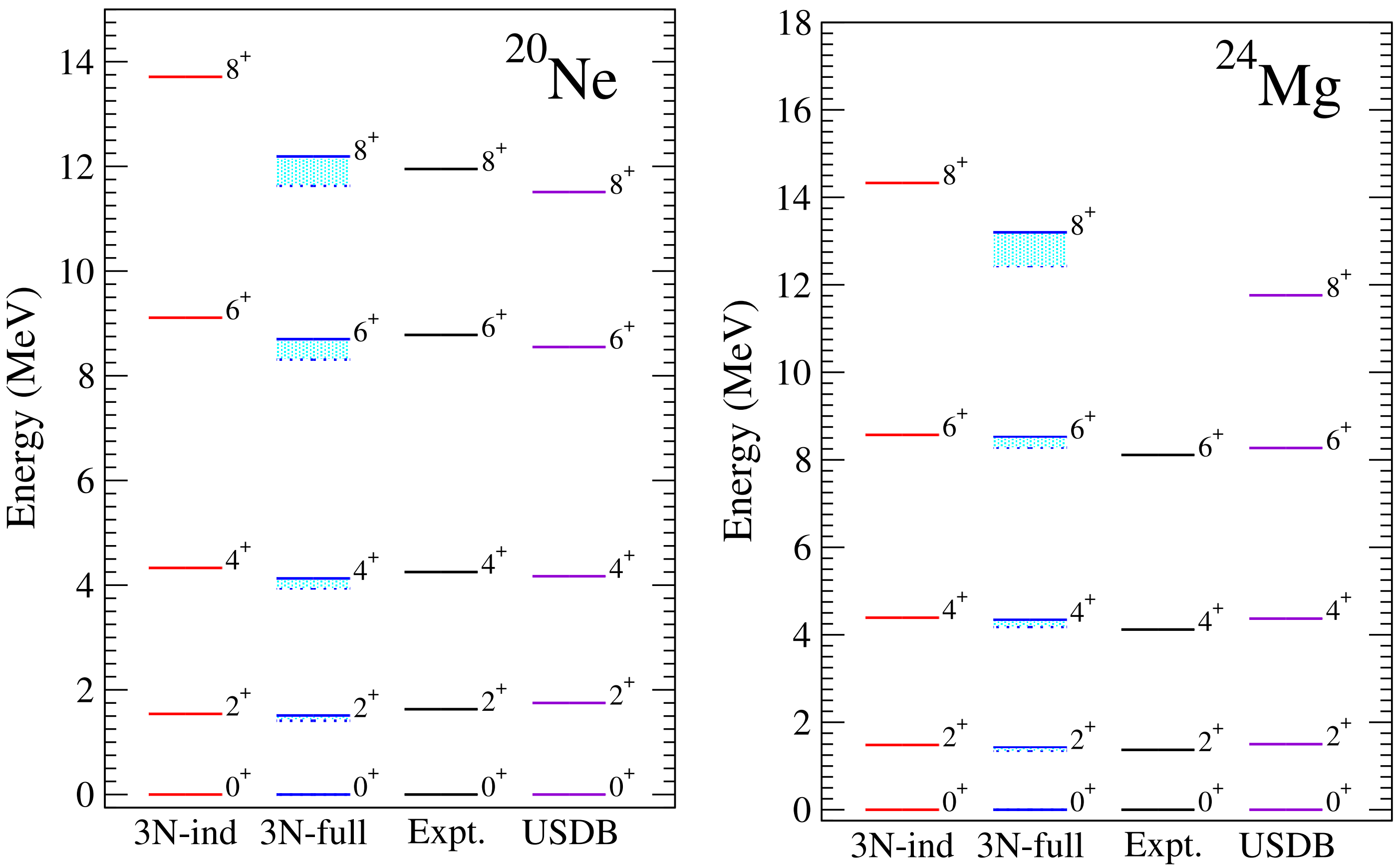
IM-SRG: **competitive with phenomenology**, good agreement with data

Deformed Systems: ^{20}Ne and ^{24}Mg

Ground-state rotational band for well-known deformed nuclei



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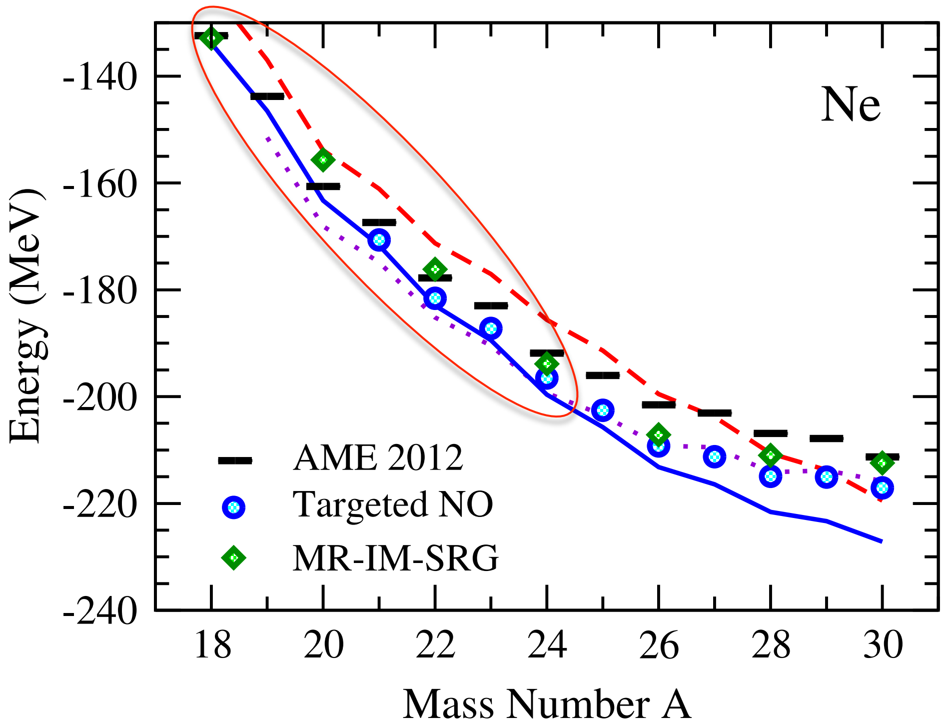
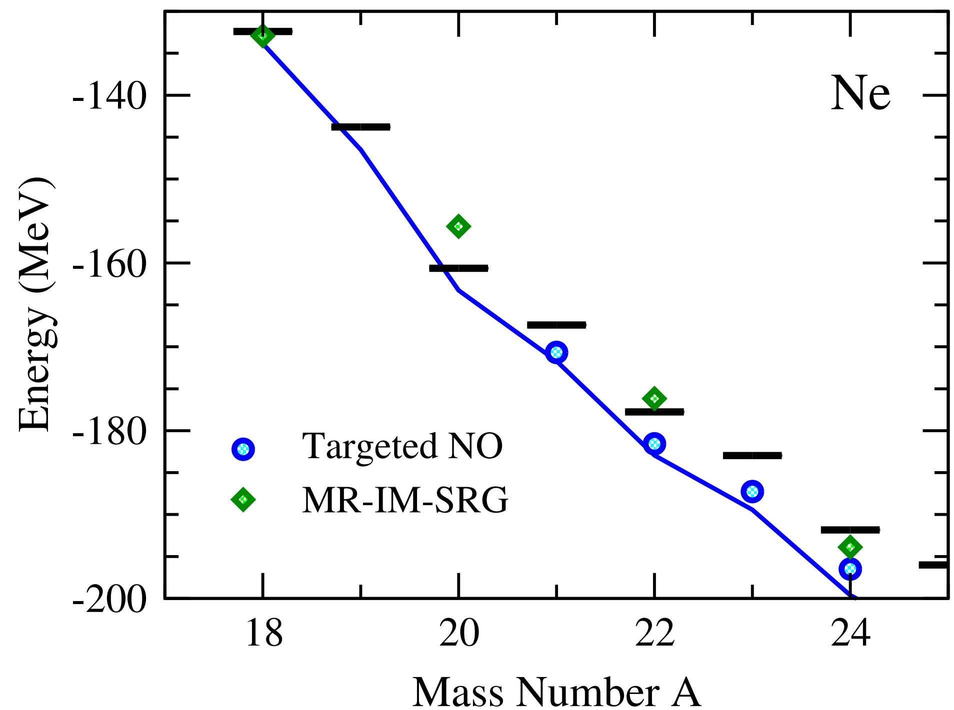
IM-SRG: **competitive with phenomenology**, good agreement with data

Further observables (quadrupole moments, E2 transitions) needed

Deformation with Large-Space MR-IM-SRG?

Ground states in light neon isotopes – clear discrepancies in ^{20,22}Ne





MR-IM-SRG built on spherical reference state

Not expected to produce deformed ground states – not a problem for SM

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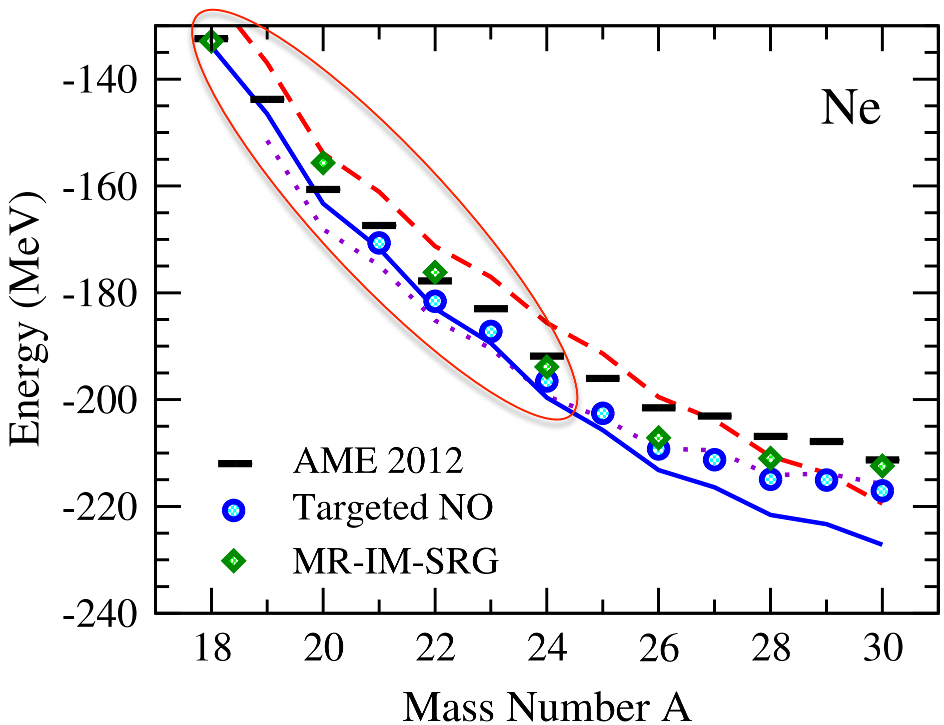
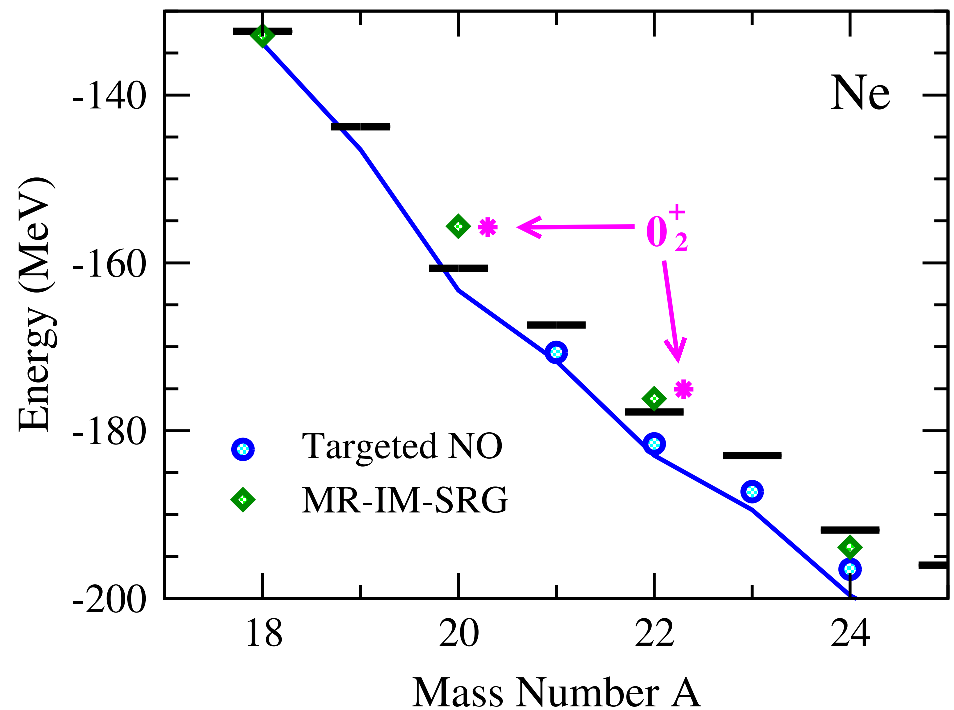




MR-IM-SRG built on spherical reference state

Not expected to produce deformed ground states – not a problem for SM

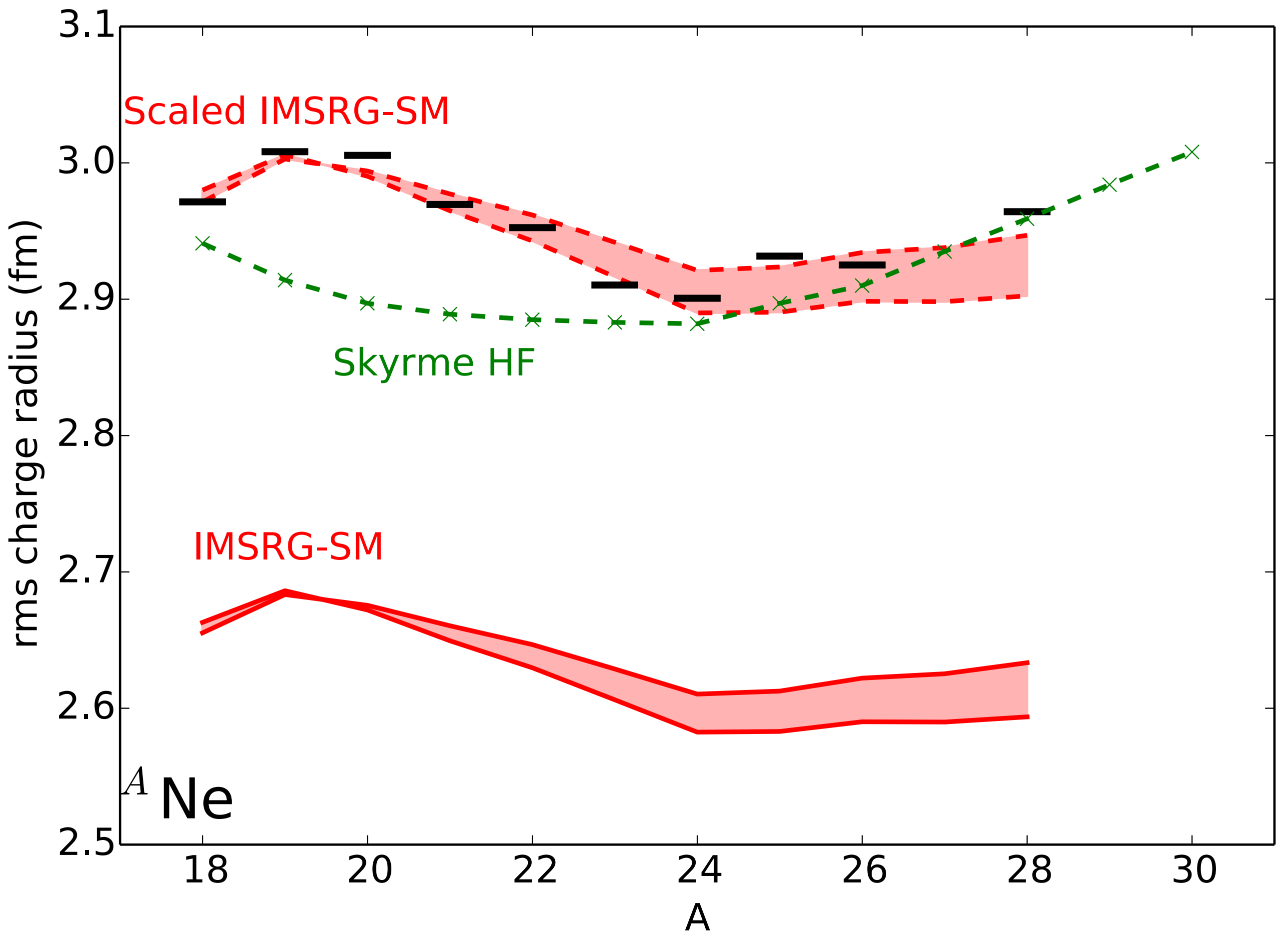
First (likely spherical) excited 0^+ SM state agrees remarkably with MR-IM-SRG

Indicates SM captures physics of deformed ground state

RMS Charge Radii in sd Shell Model

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

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



Stroberg et al., in prep

Next: general tensor operators M1, E2, GT, double-beta decay

New Directions and Outlook

Heavier semi-magic chains: MBPT as guide

Ab initio valence-shell Hamiltonians

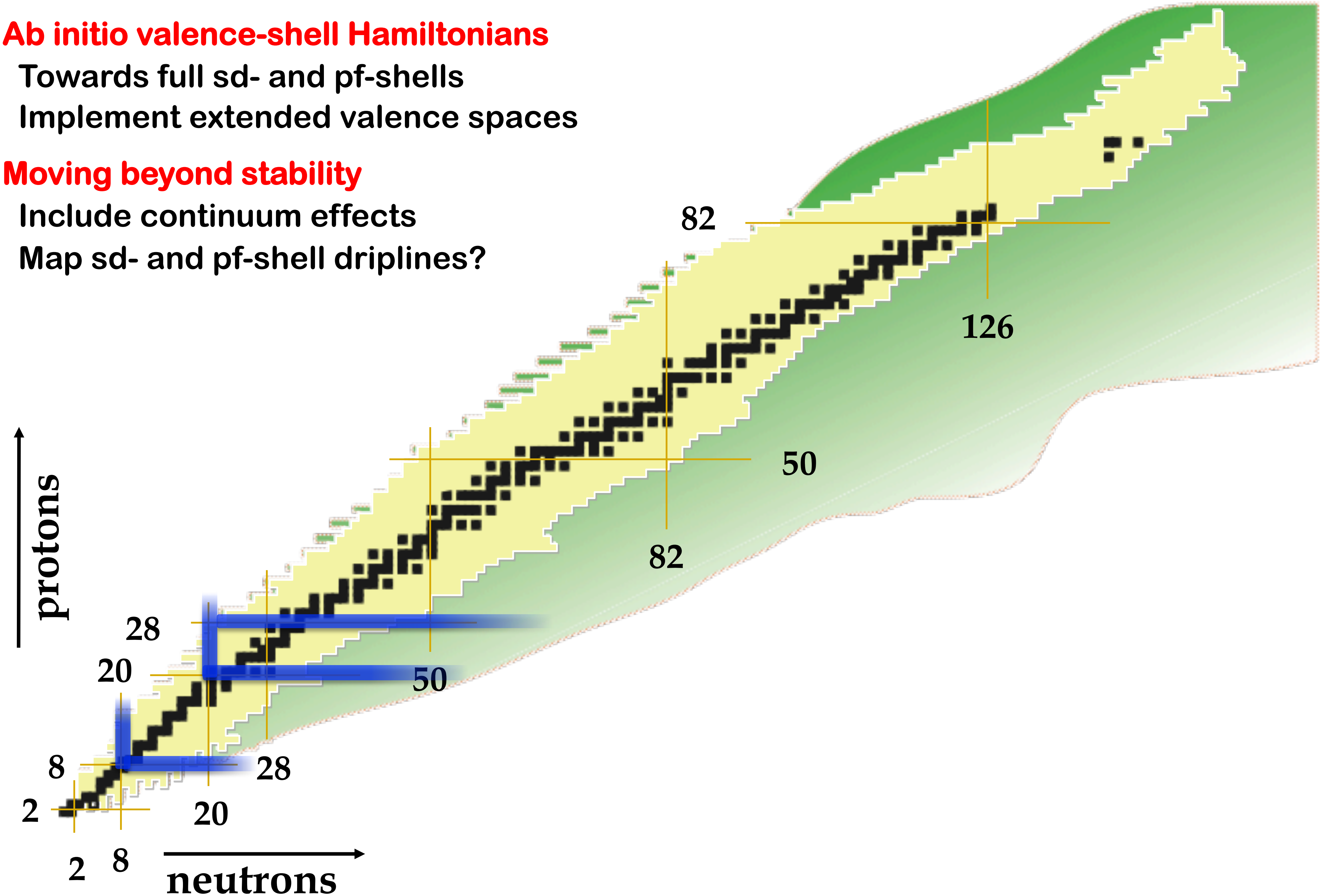
Towards full sd- and pf-shells

Implement extended valence spaces

Moving beyond stability

Include continuum effects

Map sd- and pf-shell driplines?



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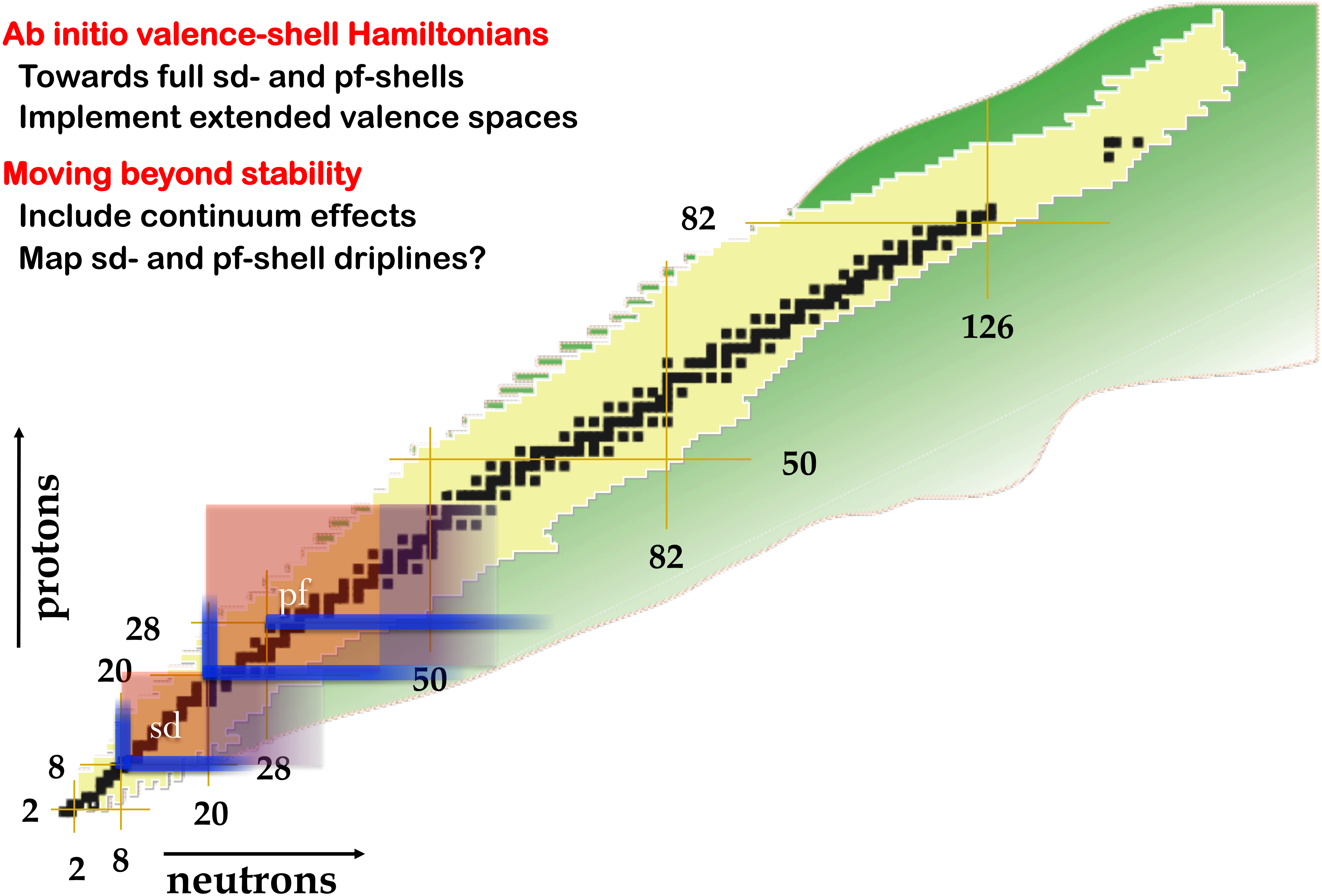


New Directions and Outlook

Heavier semi-magic chains: MBPT as guide

Ab initio valence-shell Hamiltonians

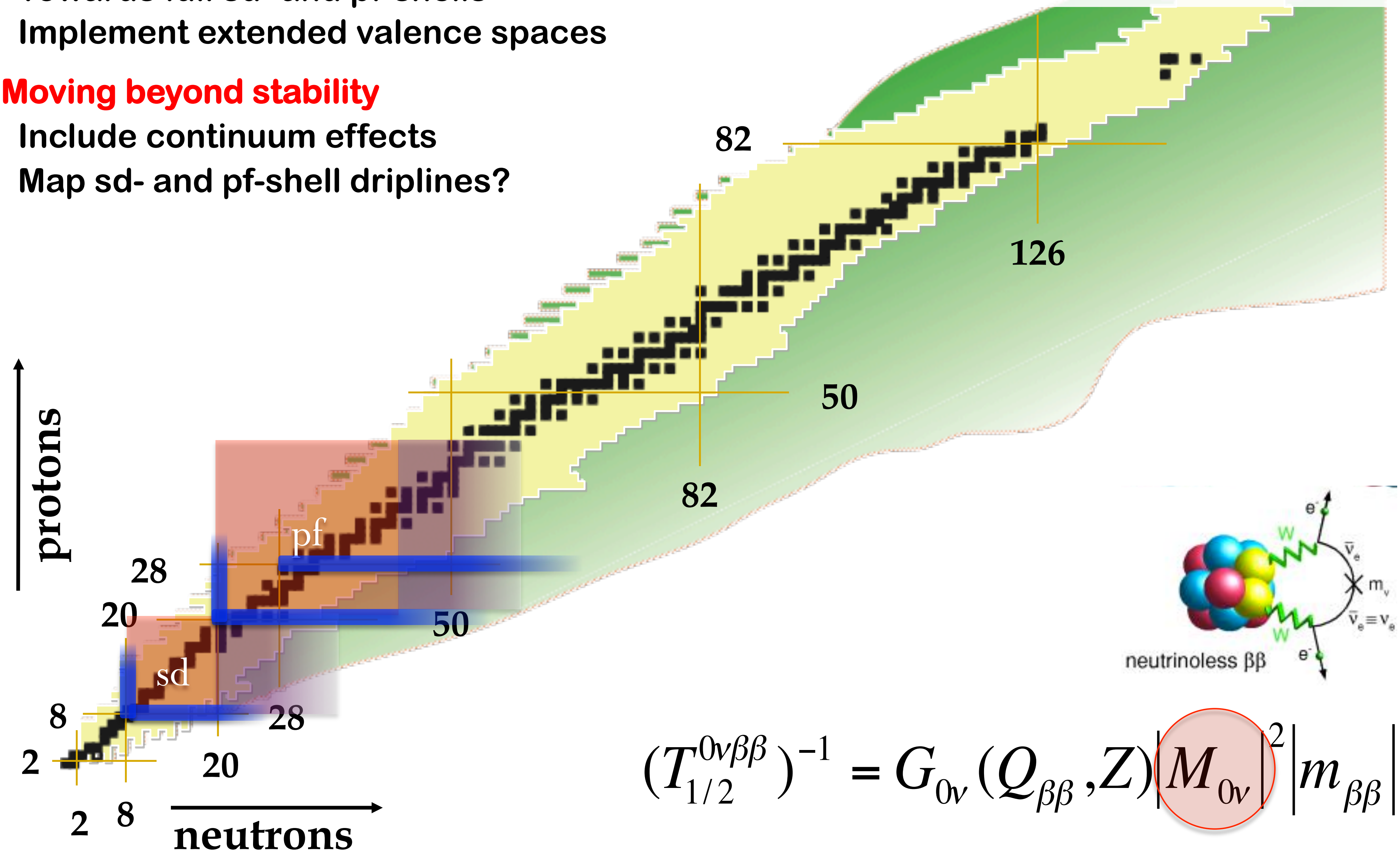
- Towards full sd- and pf-shells
- Implement extended valence spaces

Moving beyond stability

- Include continuum effects
- Map sd- and pf-shell driplines?

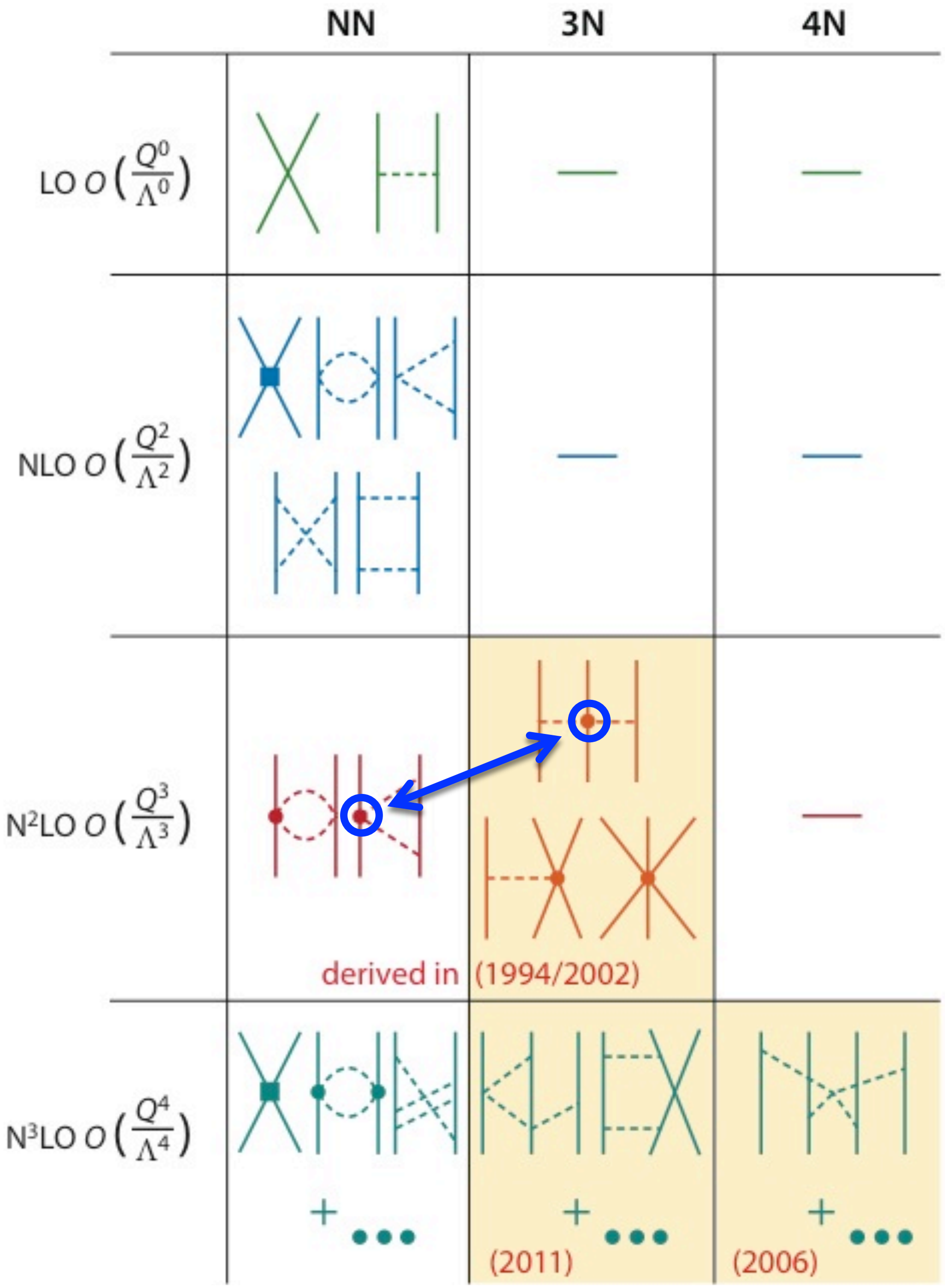
Fundamental symmetries

- Effective electroweak operators
- ab initio calculation of $0\nu\beta\beta$ decay



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

Chiral Effective Field Theory: Nuclear Forces



Weinberg, van Kolck, Kaplan, Savage, Wise…

Nucleons interact via pion exchanges and contact interactions

Consistent treatment of NN, 3N,…

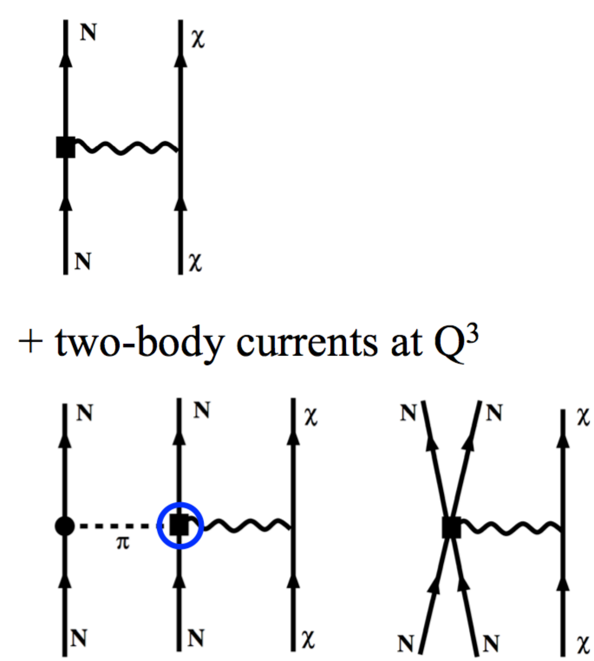
NN couplings fit to scattering data

3N couplings fit to 3/4-body systems

Consistent EW/WIMP interactions

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

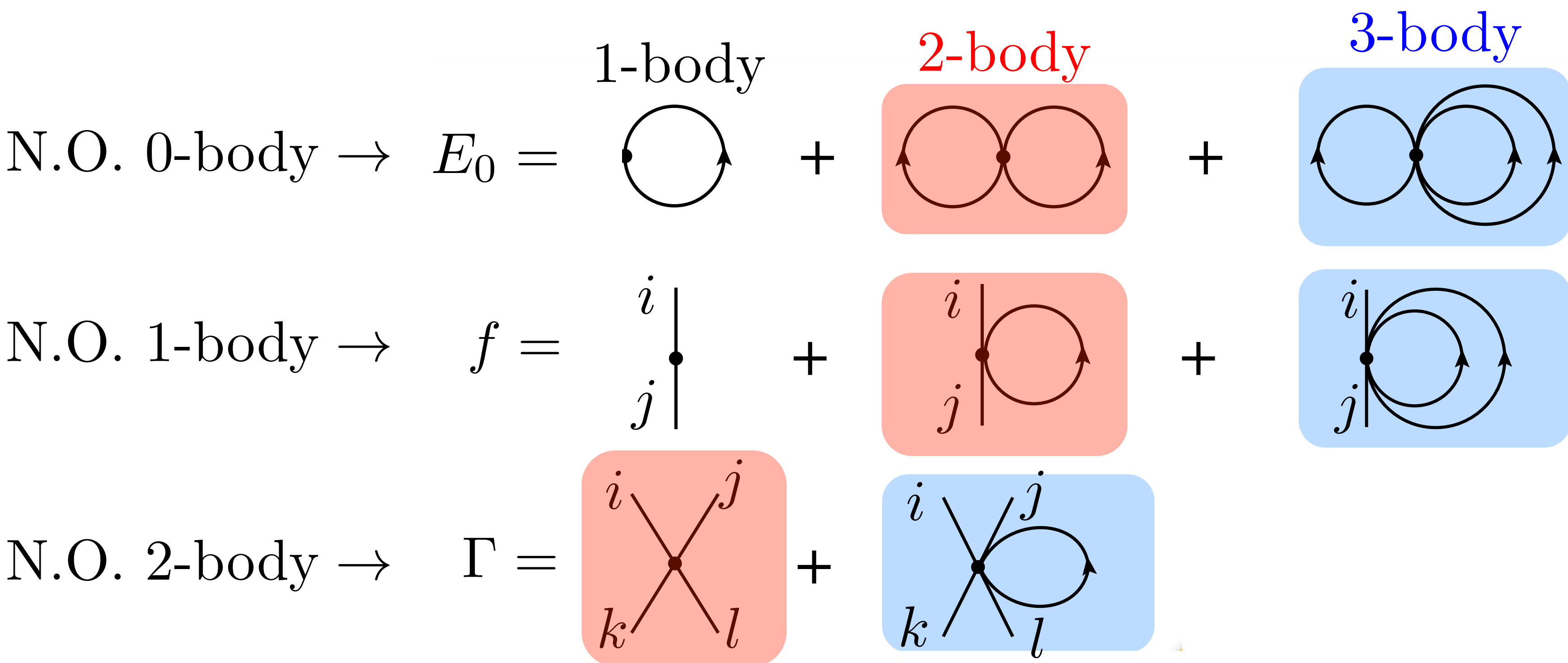
+ two-body currents at Q^3



Normal-Ordered Hamiltonian

Now rewrite exactly the initial Hamiltonian in normal-ordered form

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



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

Loop = **sum over occupied states**

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

IM-SRG: Flow Equation Formulation

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

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

chosen for desired decoupling behavior – e.g.,

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

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

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

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

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

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

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

New Approach: Magnus Expansion

Morris, **Parzuchowski**, Bogner, PRC (2015)

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

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

With flow equation:

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

Leads to commutator expression for evolved Hamiltonian

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

Nested commutator series – in practice truncate numerically

All calculations truncated at normal-ordered two-body level

Effective Operators

Keep unitary transformation from evolution of Hamiltonian

Can generalize to arbitrary operators

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

$$\Downarrow$$

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

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

First apply to scalar operators

E0 Transitions and Radii

Seldom calculated in nuclear shell model

In single HO shell:

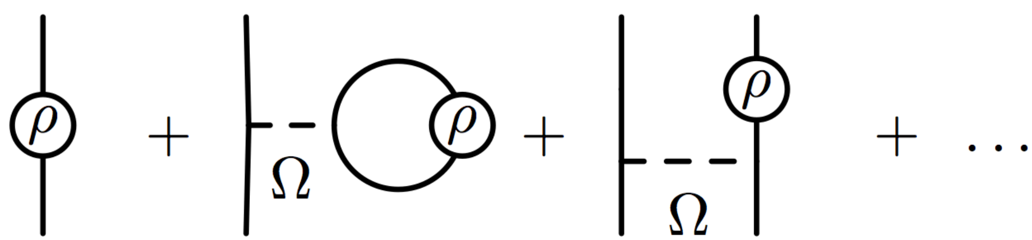
$$|\langle f|\rho_{E0}|i\rangle|^2 \propto \delta_{ij} \text{ where } \rho_{E0} = \frac{1}{e^2R}\sum_i e_i r_i^2$$

Must resort to phenomenological gymnastics

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

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

Commutators induce important higher-order and two-body parts

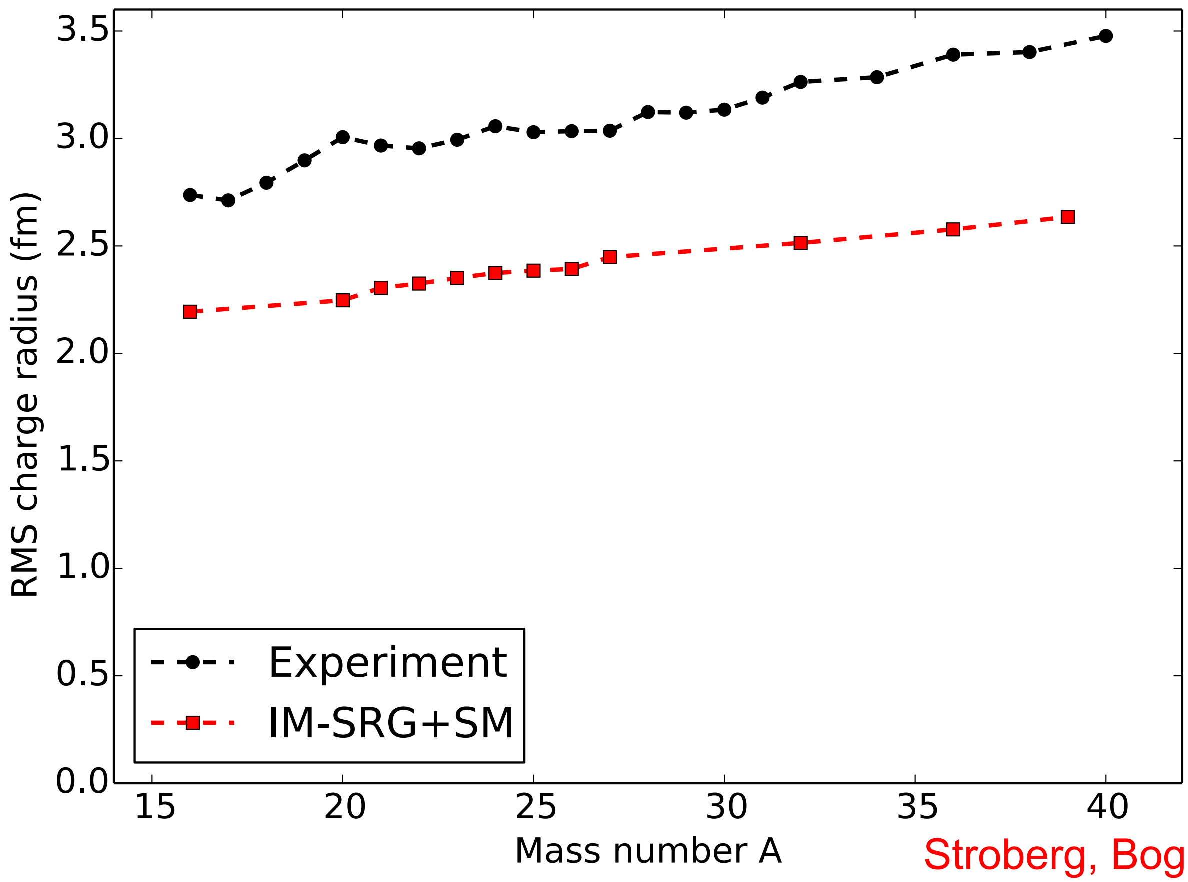


Quantify importance of induced higher-body contributions!

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

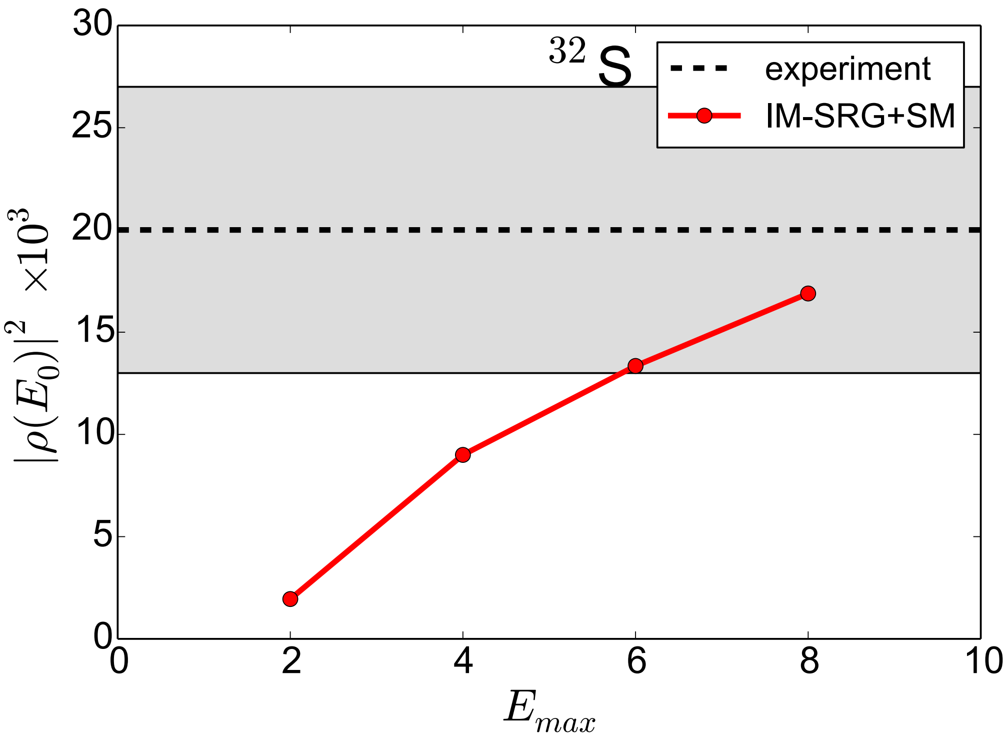
Benchmarked against NCSM in various SM codes

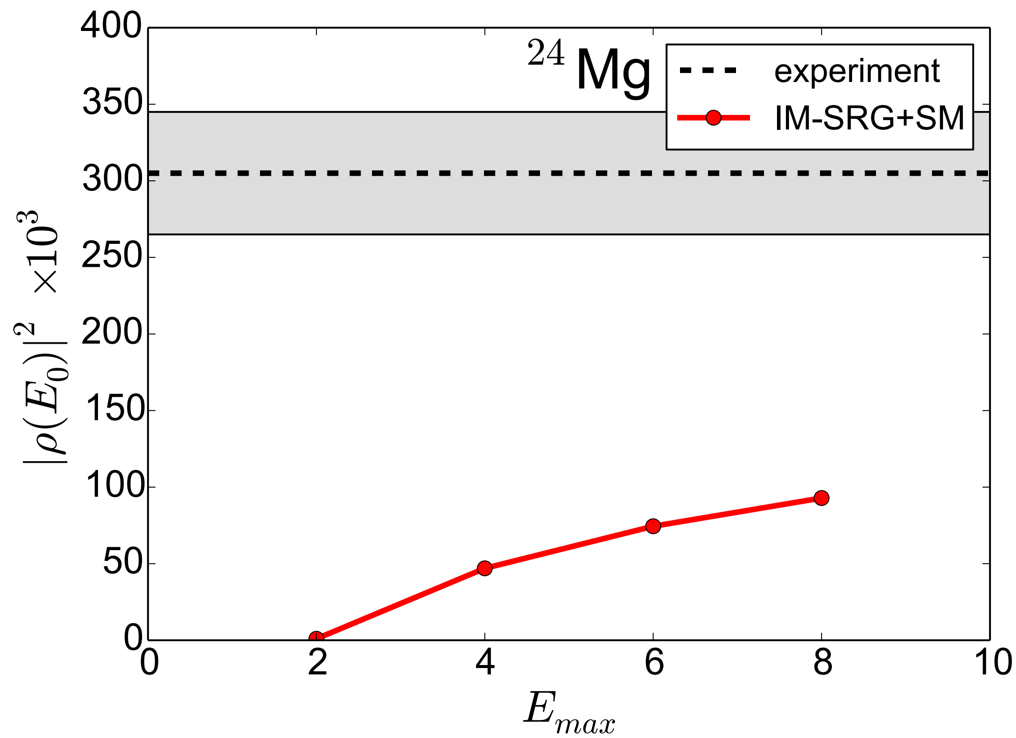
~10% too small – deficiencies expected to come from initial Hamiltonian

Two-body part important 15-20%

E0 Transitions in sd Shell Model

Preliminary results in *sd* shell:

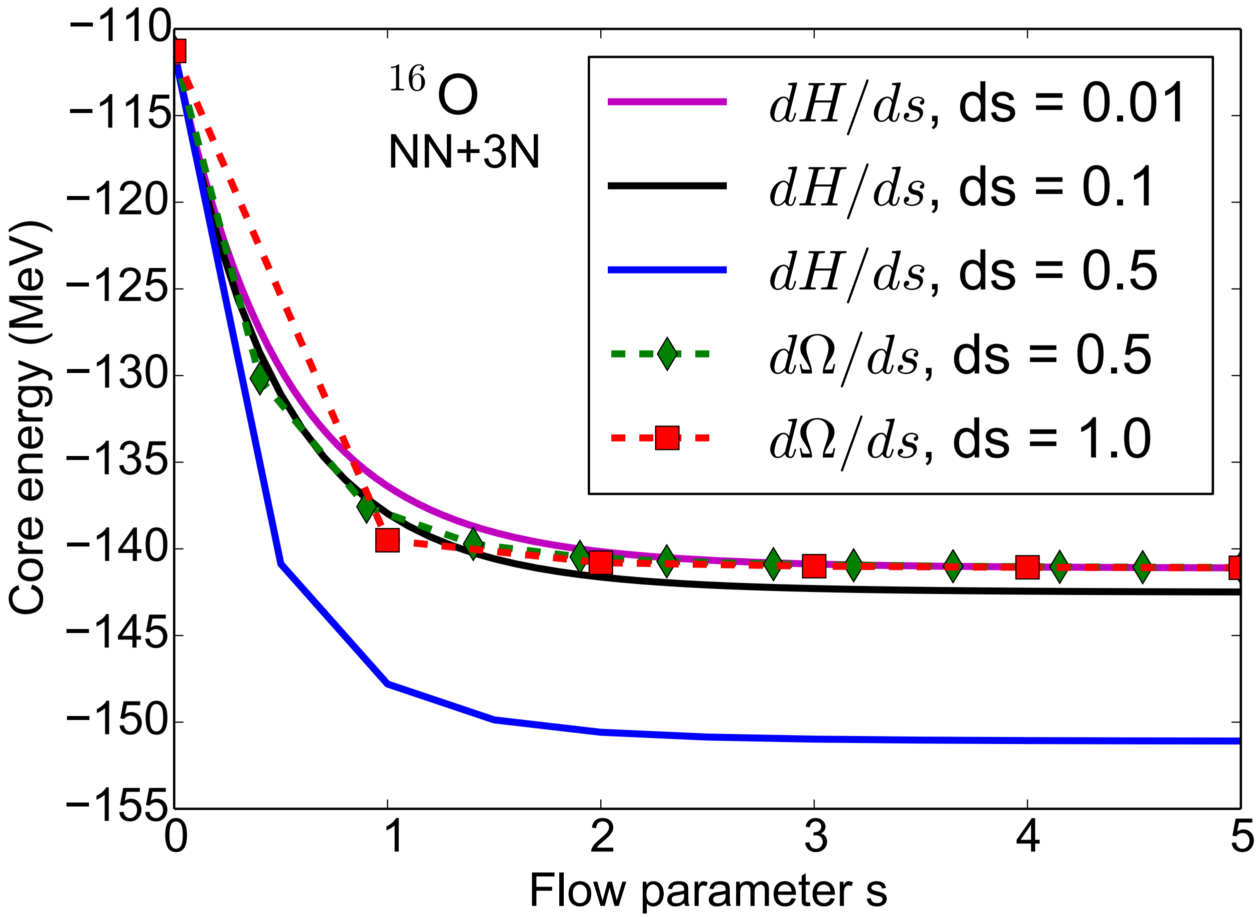




Promising but need additional benchmarks

Magnus vs Flow-Equation

Variation of step size

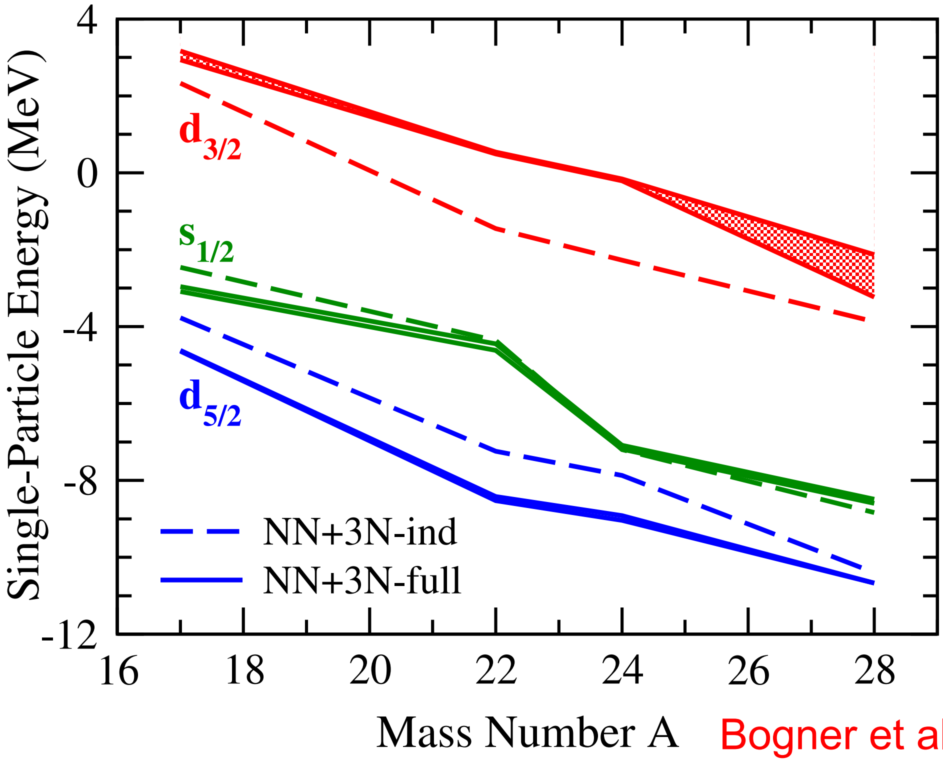


Evident error accumulation in flow-equation for small step sizes

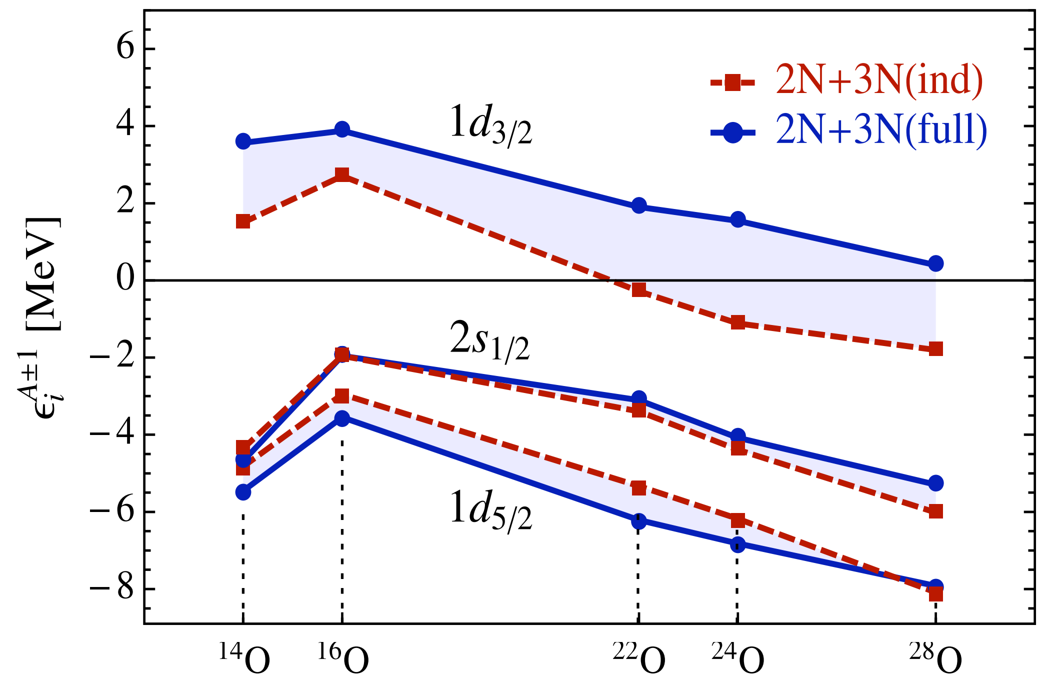
Magnus: rapid convergence, independent of step size

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

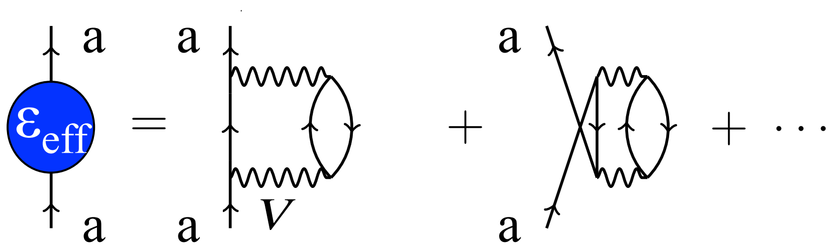
Perturbative Approach

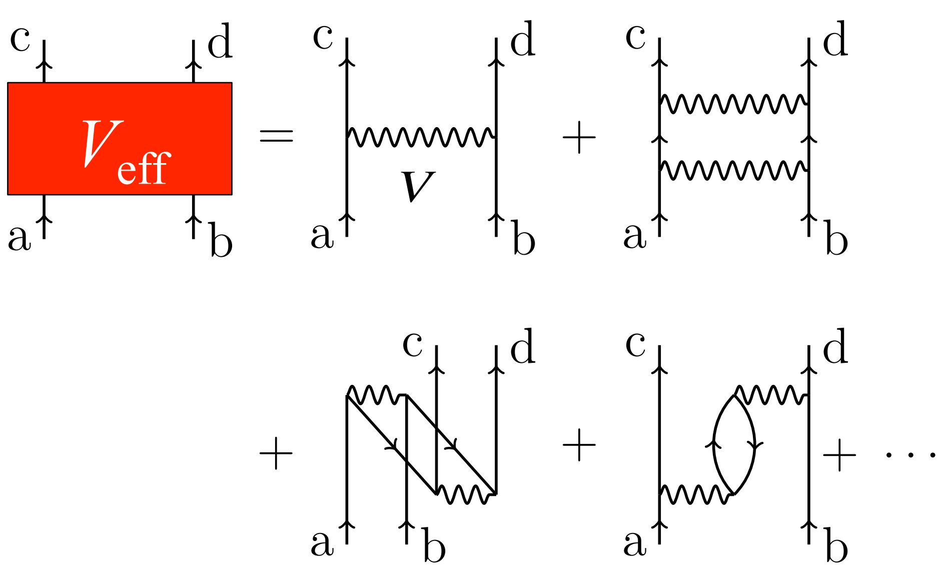
1) Effective Hamiltonian: sum excitations outside valence space to **MBPT(3)**

2) Self-consistent single-particle energies

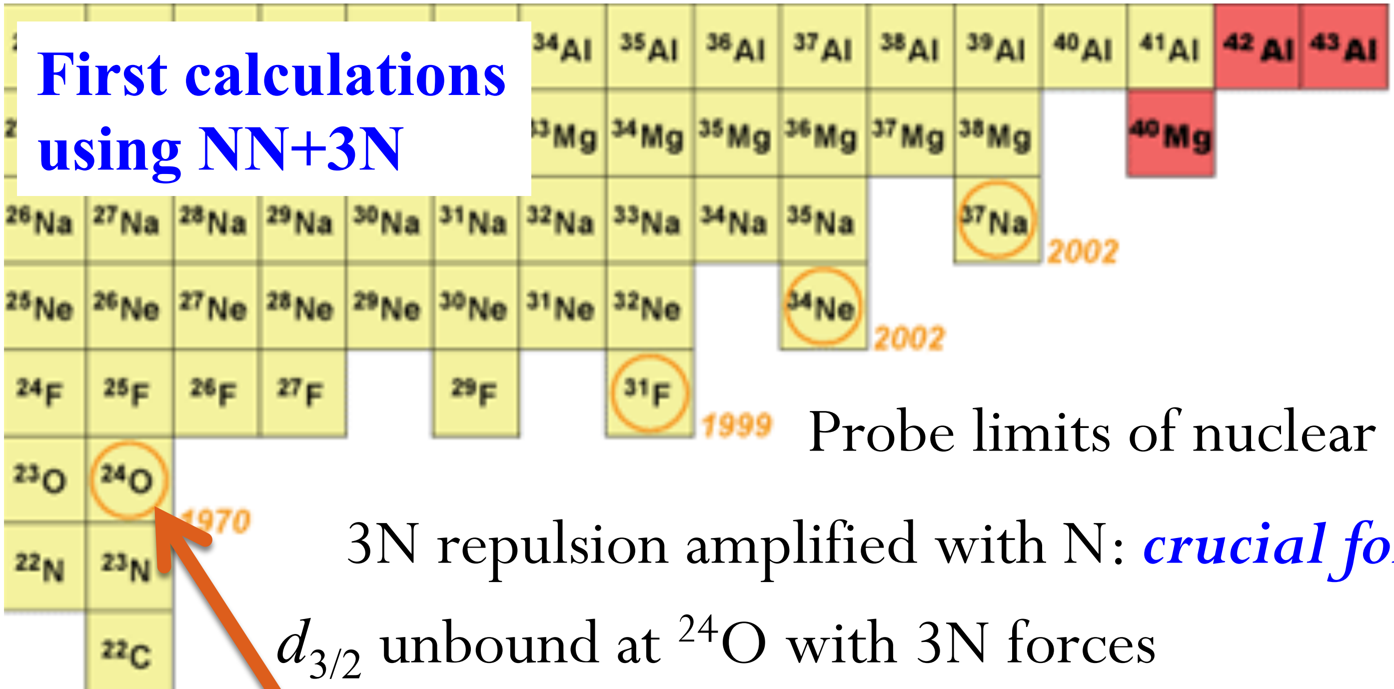
3) **Harmonic-oscillator** basis of 13-15 major shells: **converged**

4) NN and 3N forces from chiral EFT





Oxygen Anomaly

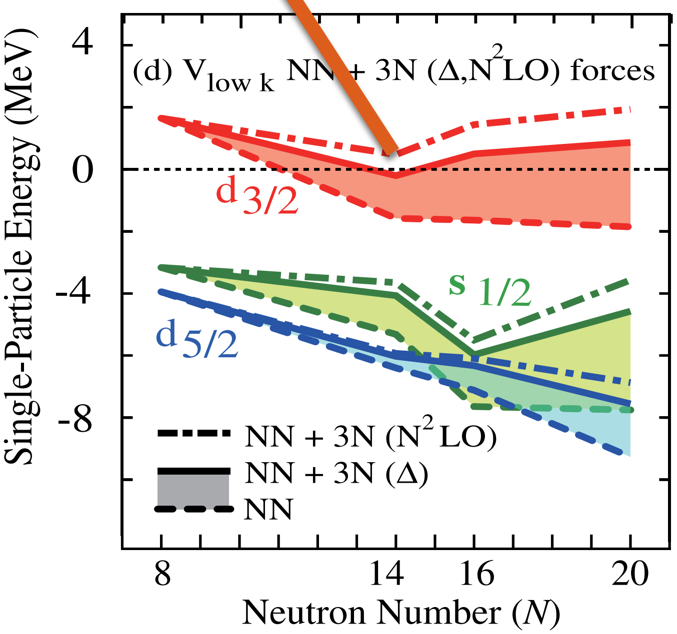


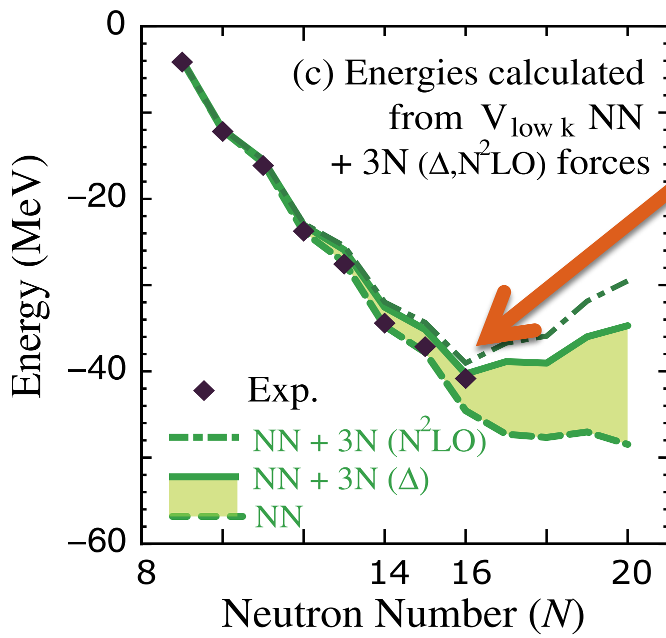
First calculations using NN+3N

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





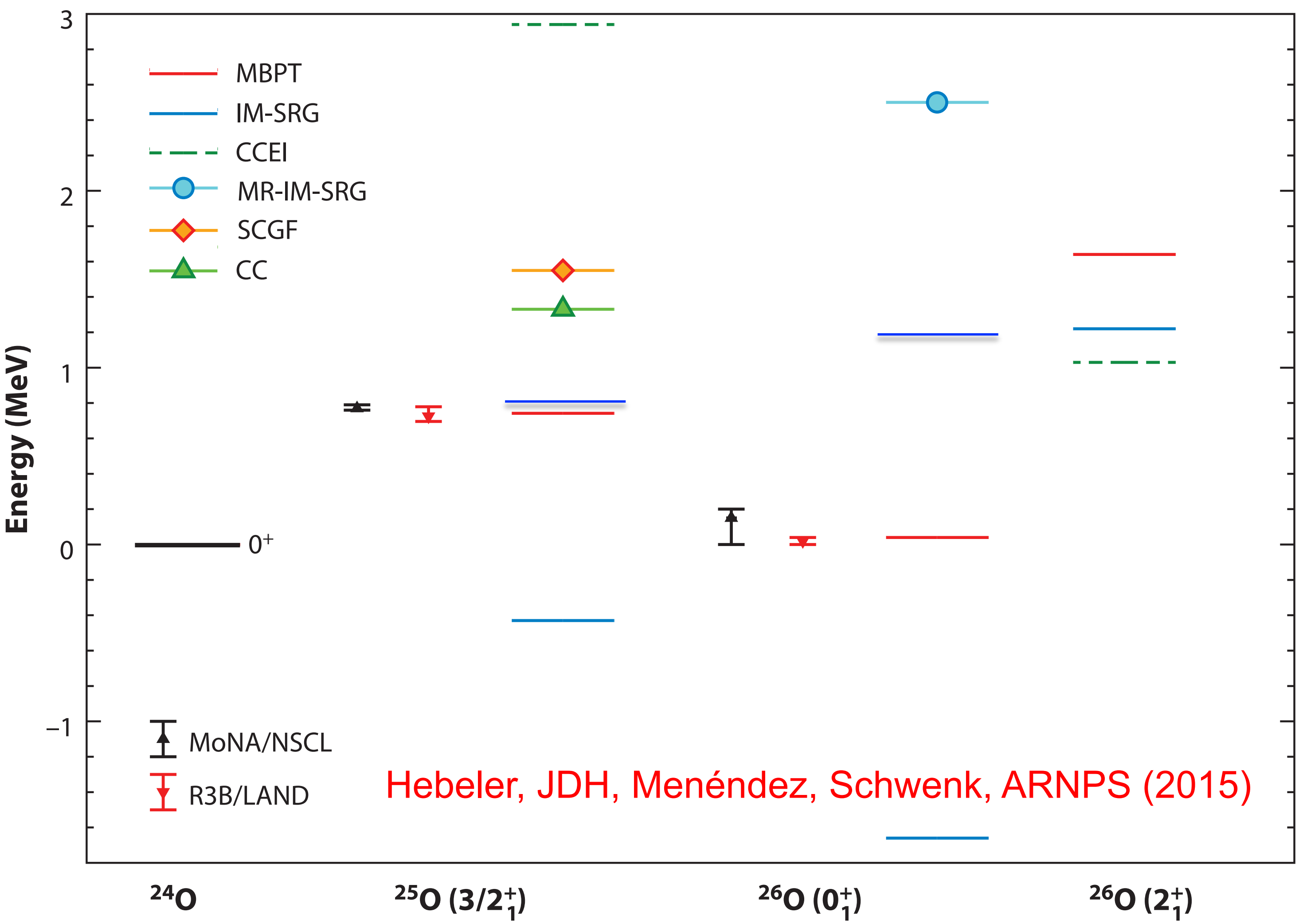
Isotopes unbound beyond ^{24}O

First microscopic explanation of oxygen anomaly

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

Beyond the Oxygen Dripline

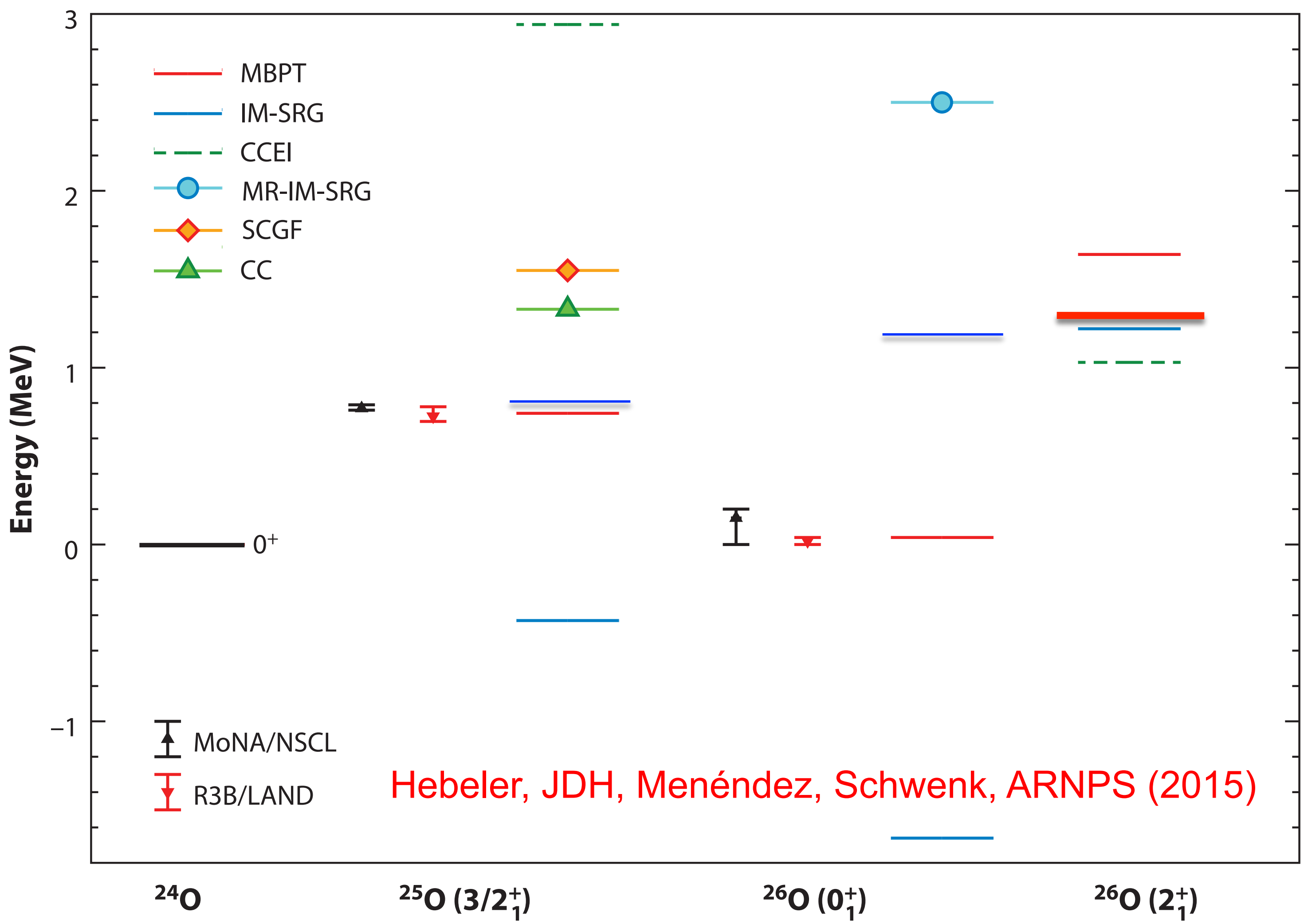
Physics beyond dripline highly sensitive to 3N forces and continuum effects



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

Beyond the Oxygen Dripline

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

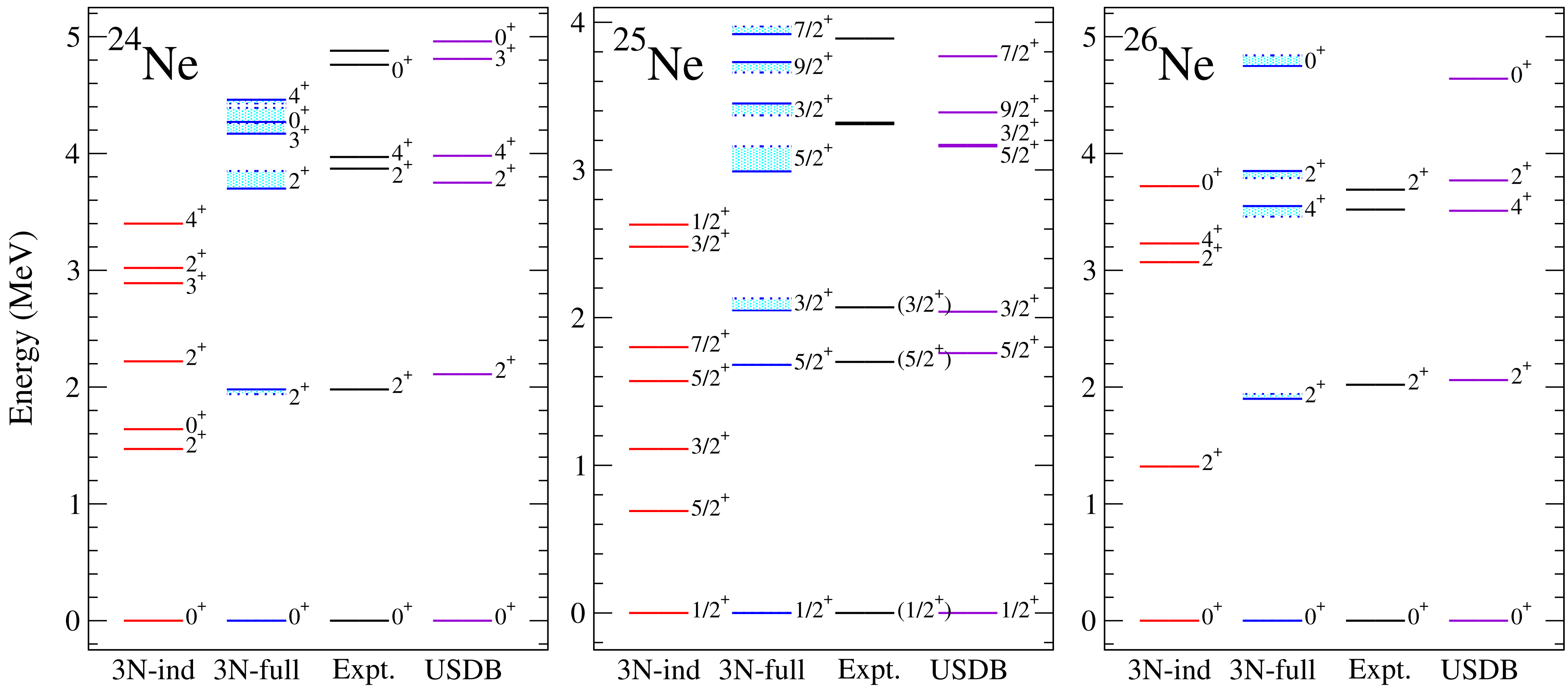


Kondo et al, preliminary

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

Doubly Open Shell: Neutron-Rich Ne Spectra

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



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

NN+3N-ind: clear deficiencies

NN+3N-full: **competitive with phenomenology**, good agreement with data

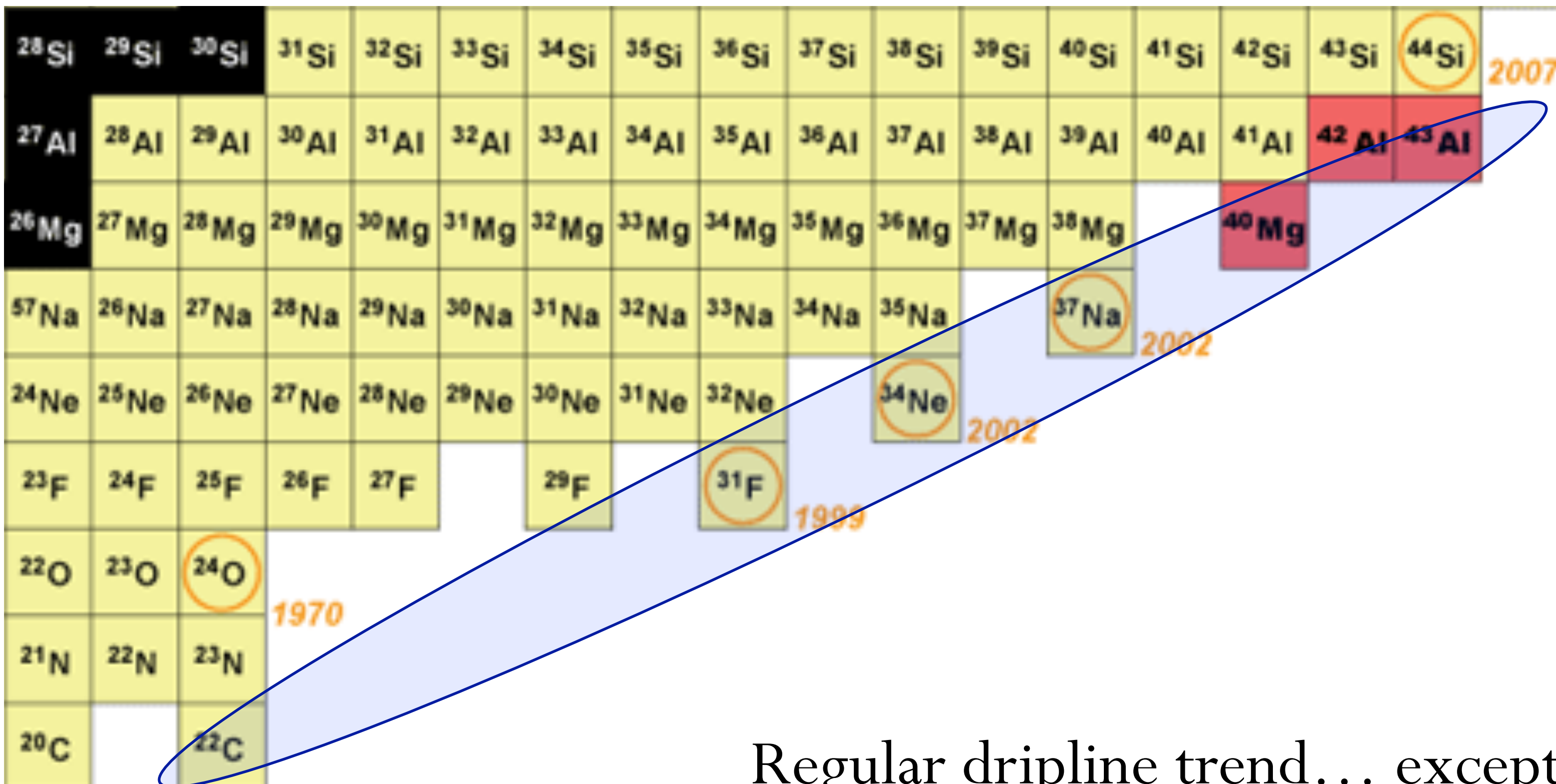
Limits of Nuclear Existence: Oxygen Anomaly

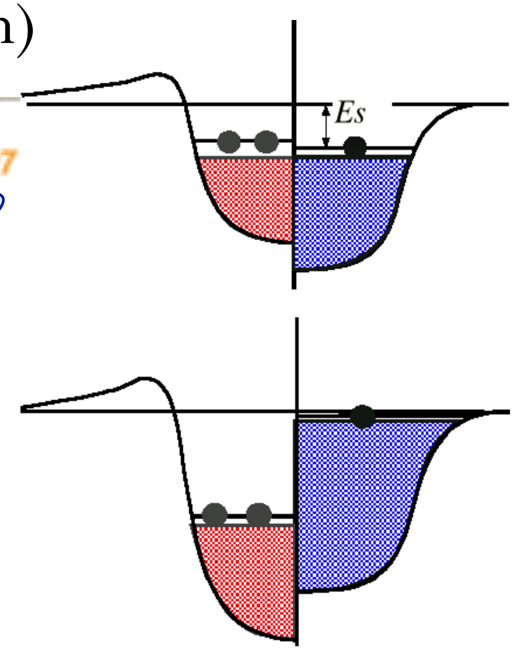
Where is the nuclear dripline?

Limits defined as last isotope with positive neutron separation energy

- Nucleons “drip” out of nucleus

Neutron dripline experimentally established to Z=8 (Oxygen)



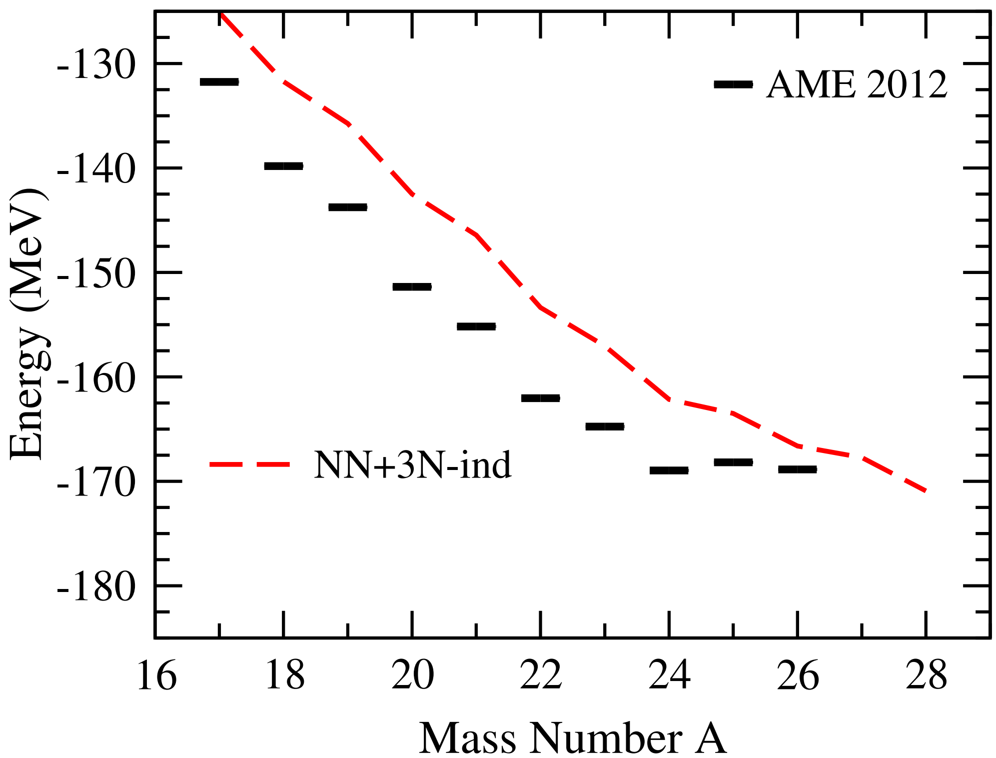


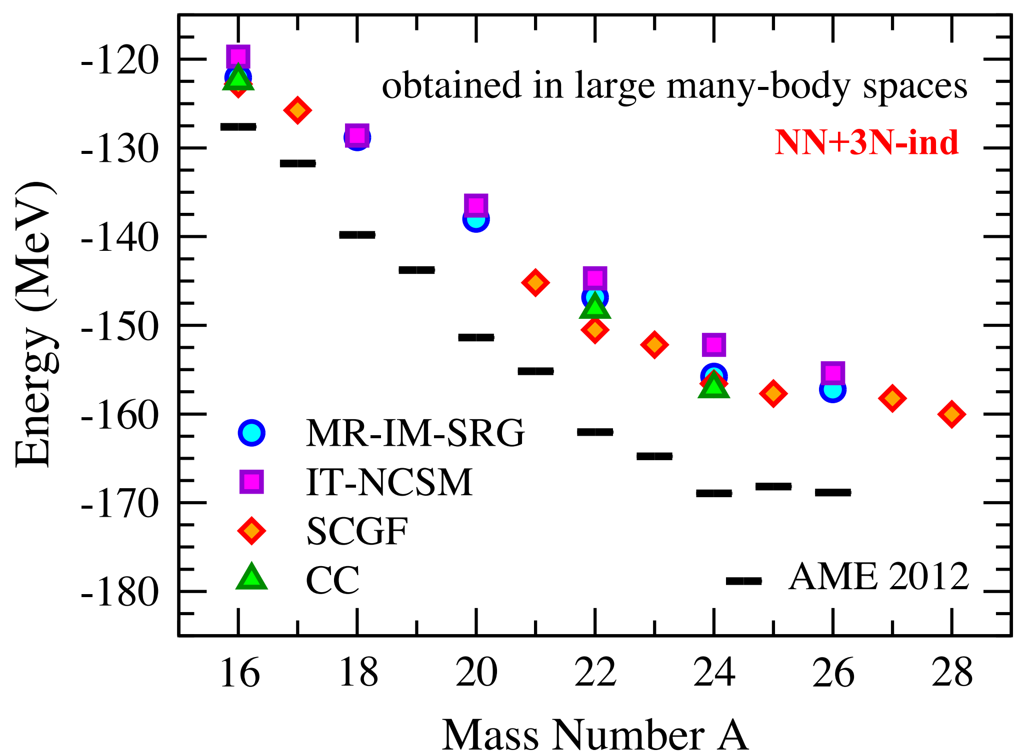
Regular dripline trend… except anomalous oxygen

Adding one proton binds 6 additional neutrons

Ground-State Energies in Oxygen Isotopes

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





Agreement between all methods with same input forces

No reproduction of oxygen dripline in any case