Ab Initio Interactions and Operators for the sd Valence-Space

Jason D. Holt

NSERC CRSNG

TRIUMF

NRC·CNRC

TRIUMF THE UNIVERSITY OF BRITISH COLUMBIA

R. Stroberg

D. Fullerton

P. Navratil

MICHIGAN STATE UNIVERSITY

S. Bogner H. Hergert

TECHNISCHE UNIVERSITÄT DARMSTADT

A. Schwenk

東京大学 THE UNIVERSITY OF TOKYO

J. Menendez

The Nuclear Many-Body Problem

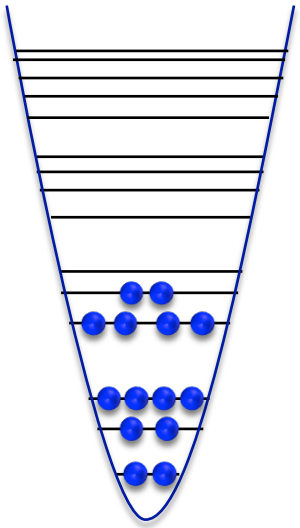
Nucleus strongly interacting many-body system – A-body problem impossible

$$H\psi_n = E_n\psi_n$$

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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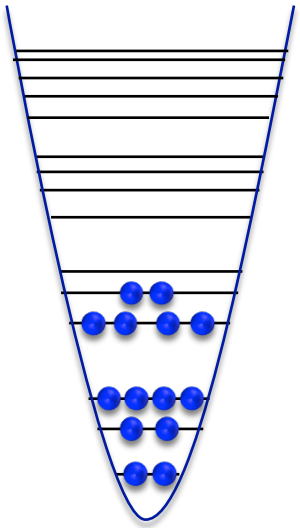

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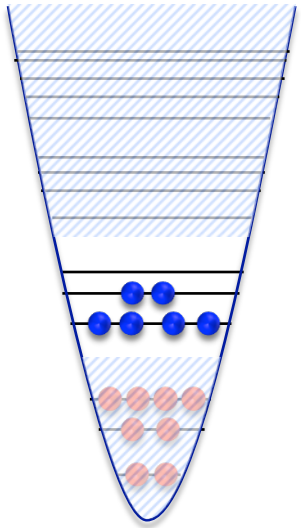

All nuclei near closed-shell cores

All properties:

Ground states

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EW transitions

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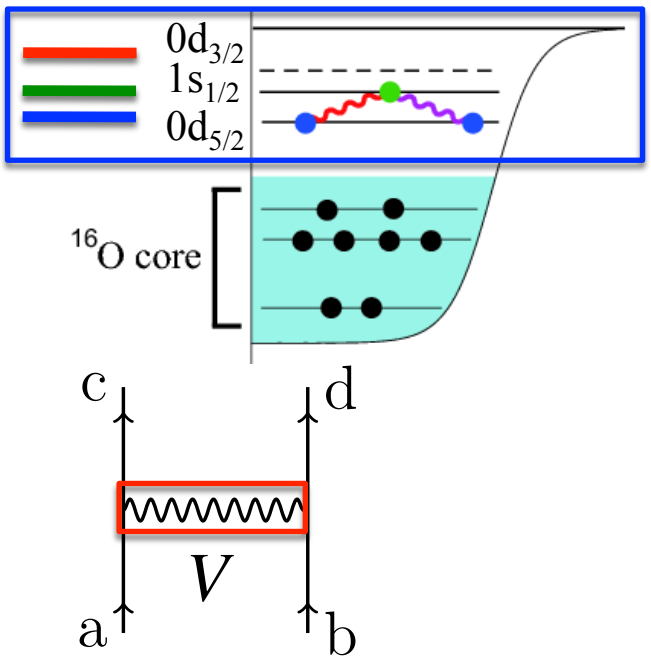
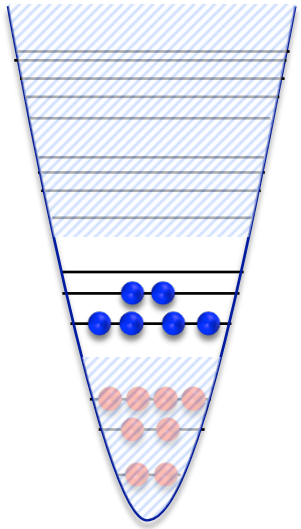
$$H_{\text{v.s.}} = \sum_i \varepsilon_i a_i^\dagger a_i + V_{\text{v.s.}}$$



Valence-space approach



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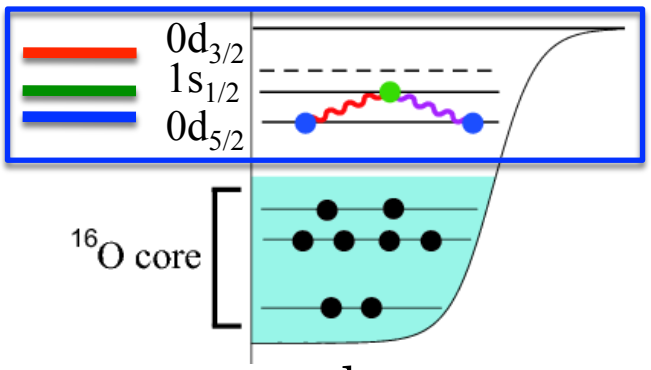
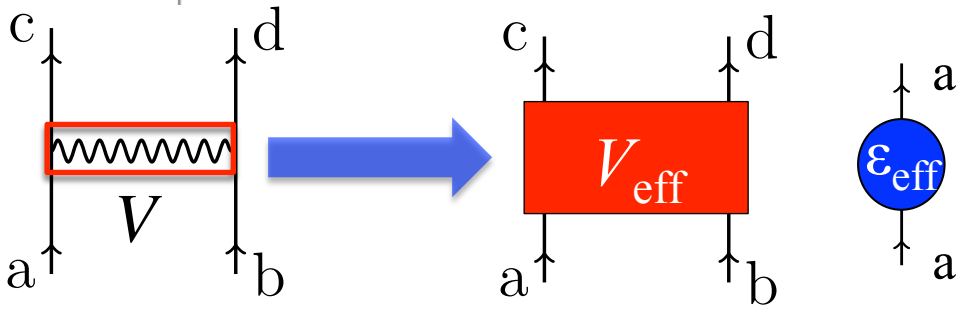
$$H_{\text{eff}} = \sum_i \varepsilon_{i_{\text{eff}}} a_i^\dagger a_i + V_{\text{eff}}$$





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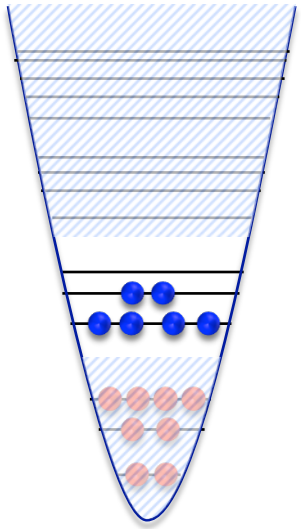

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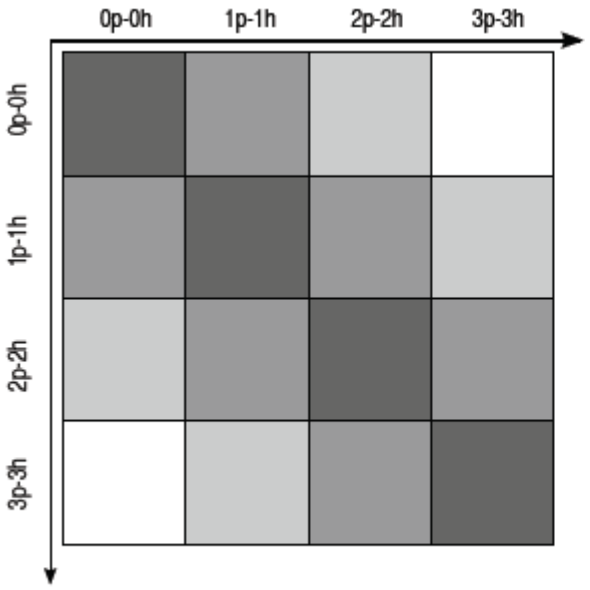
In-Medium Similarity Renormalization Group

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

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

Interaction in new basis is simple

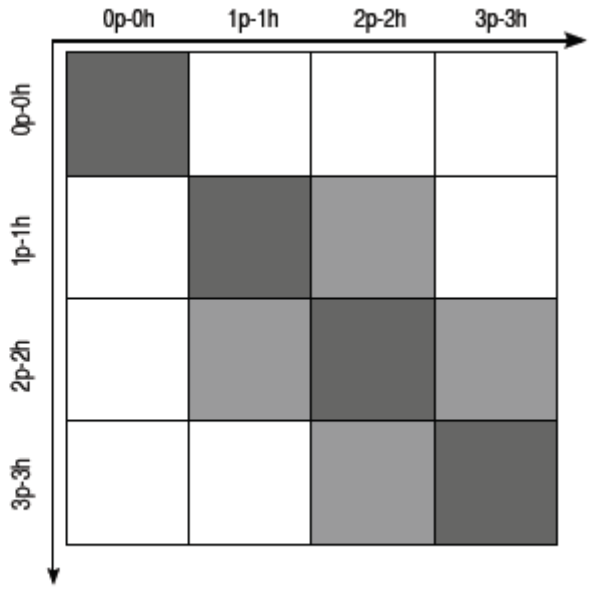
$$H^{\rm od} = \langle p|H|h\rangle + \langle pp|H|hh\rangle + \cdots + \text{h.c.}$$



$\langle i|H|j\rangle$

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

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



$$\langle {\rm n}p{\rm n}h|\tilde{H}|\Phi_0\rangle = 0$$

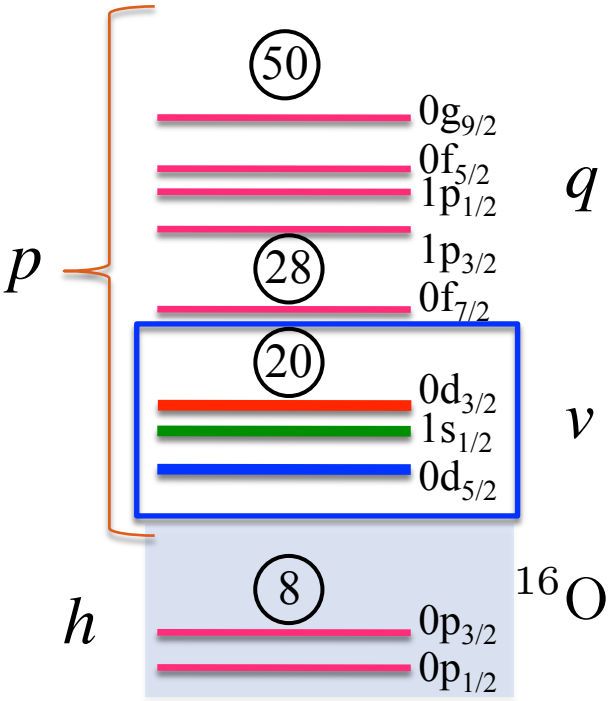
$$E_{\rm g.s} = \langle\Phi_0|\tilde{H}|\Phi_0\rangle$$

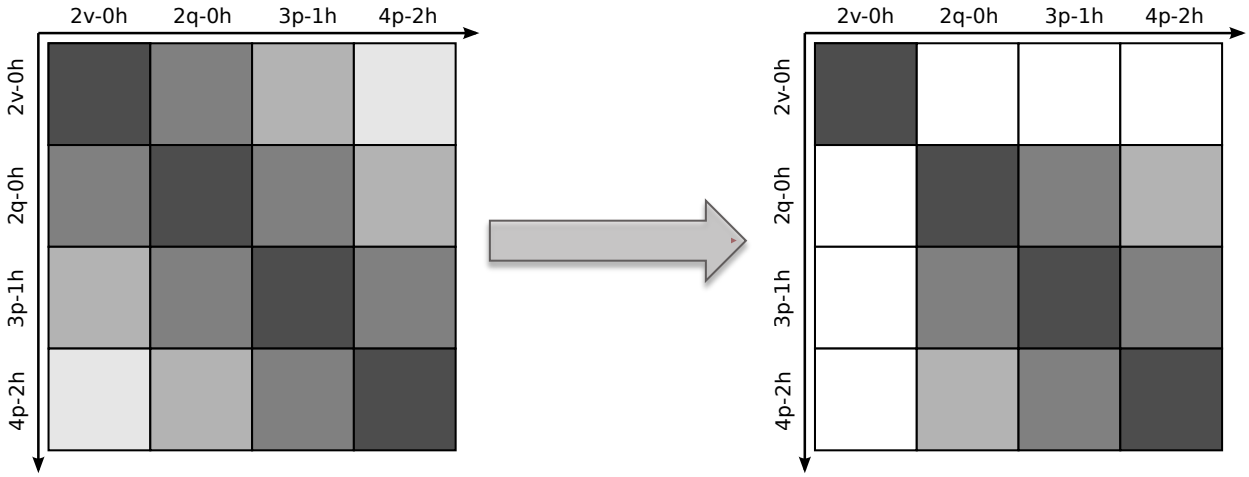
Tsukiyama, **Bogner**, Schwenk, PRL (2011)

IM-SRG for Valence-Space Hamiltonians

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

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





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

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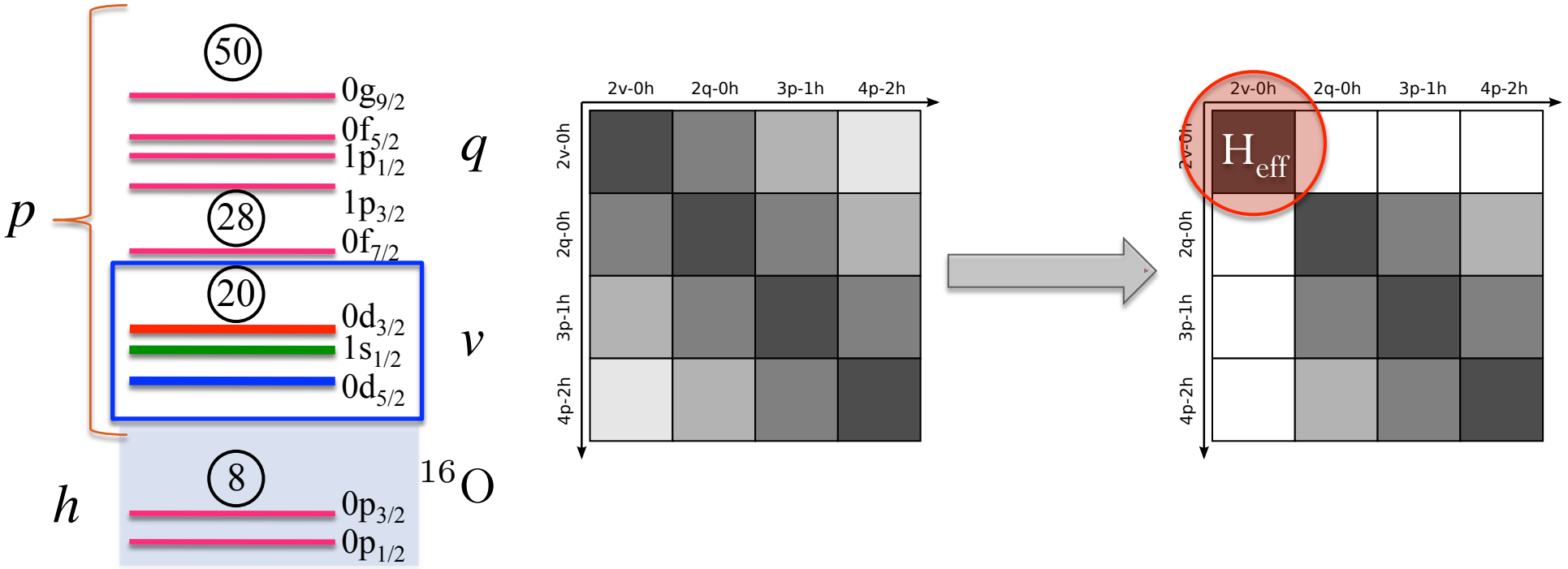
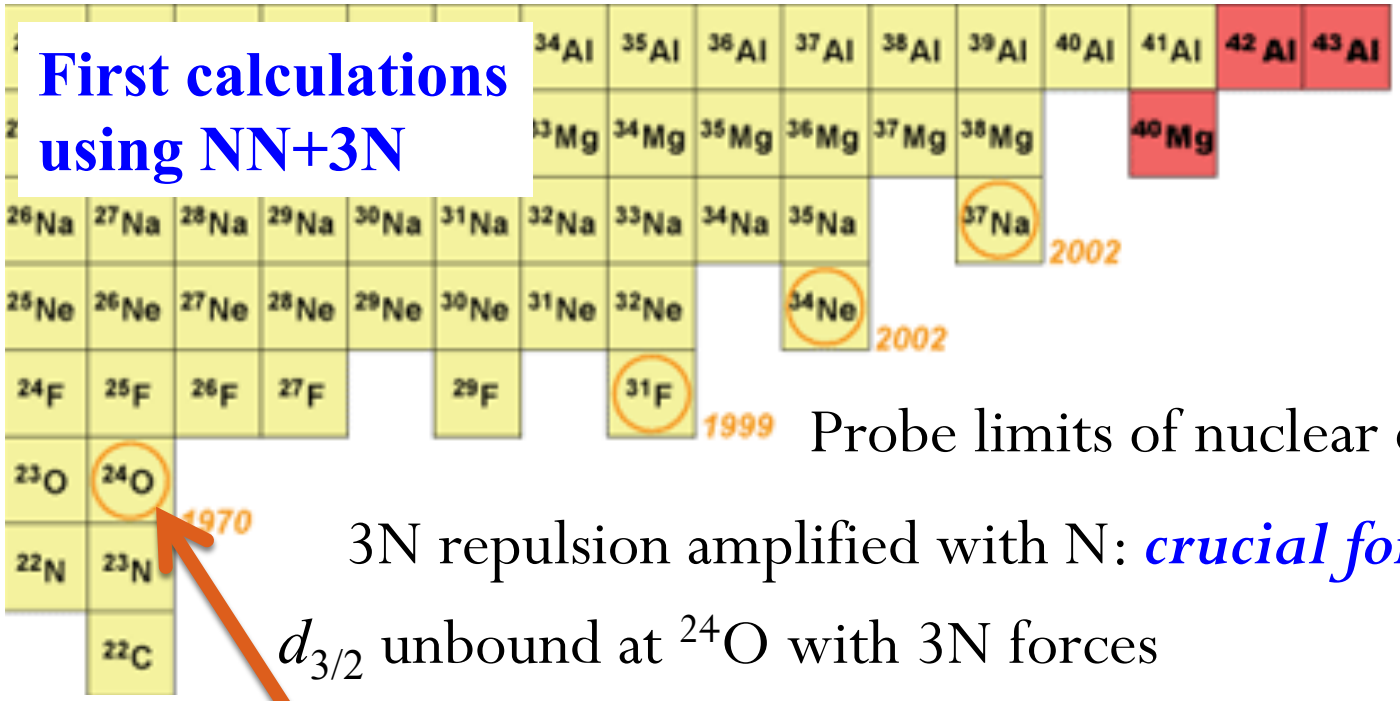


Redefine $H^{\rm od}$ to **decouple valence space from excitations** outside v

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

Oxygen Anomaly

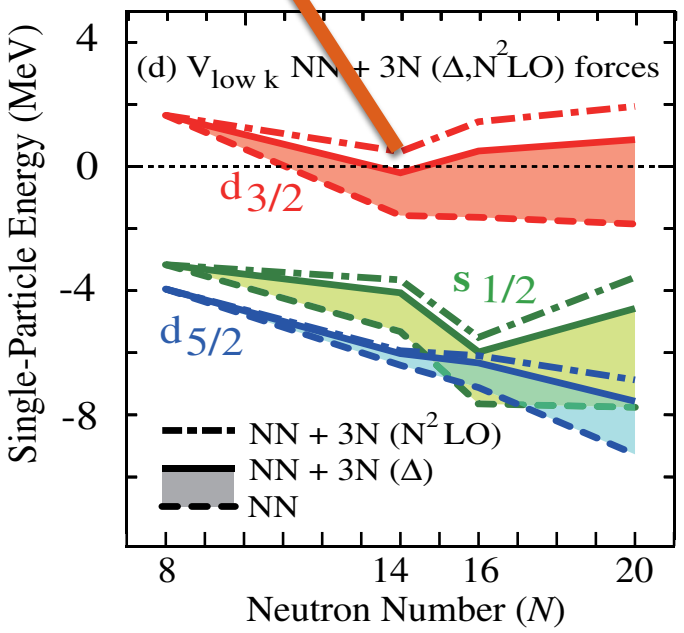
First calculations using NN+3N

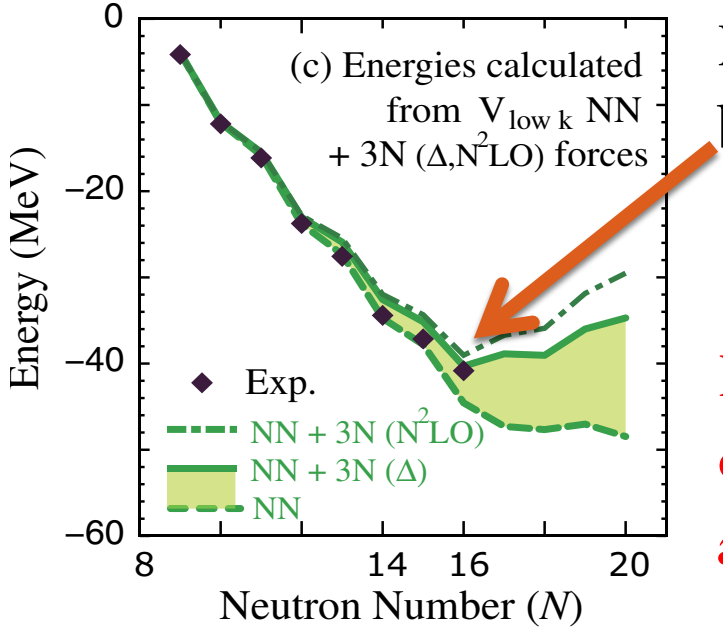


Probe limits of nuclear existence with 3N forces

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

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





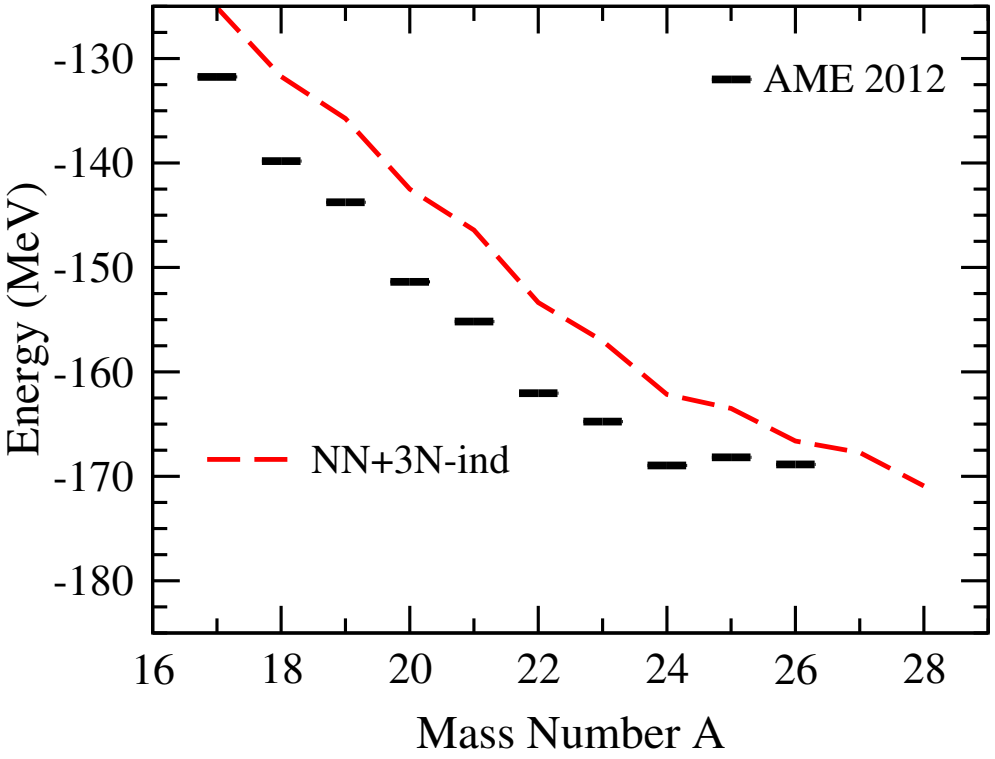
Isotopes unbound beyond ^{24}O

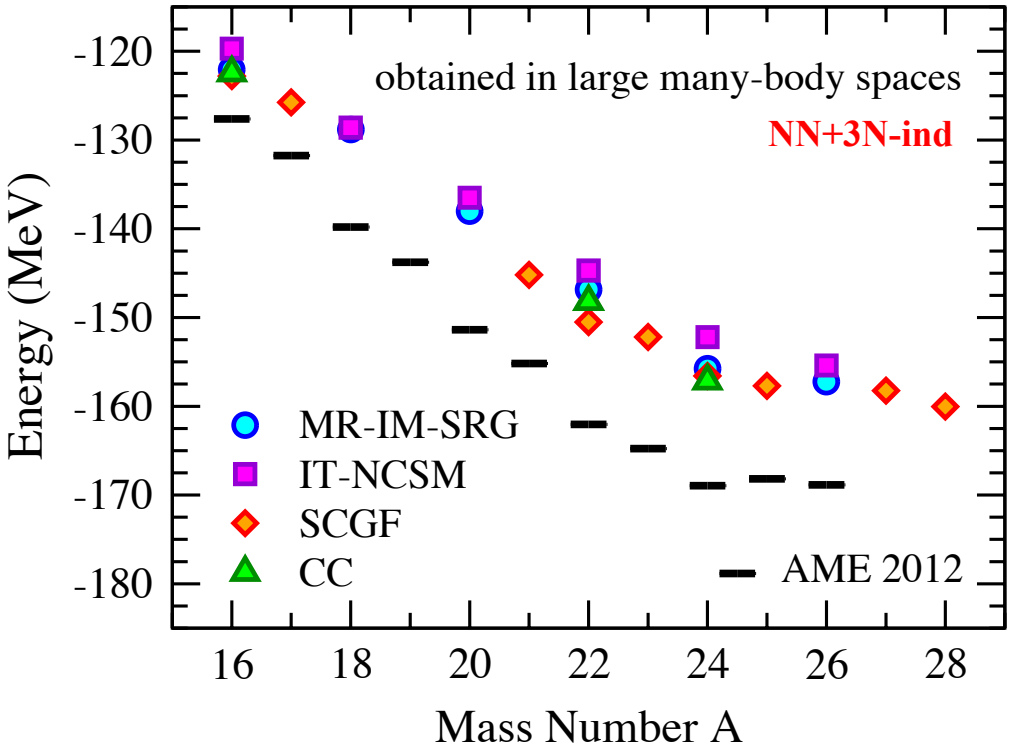
First microscopic explanation of oxygen anomaly

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

Ground-State Energies in Oxygen Isotopes

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



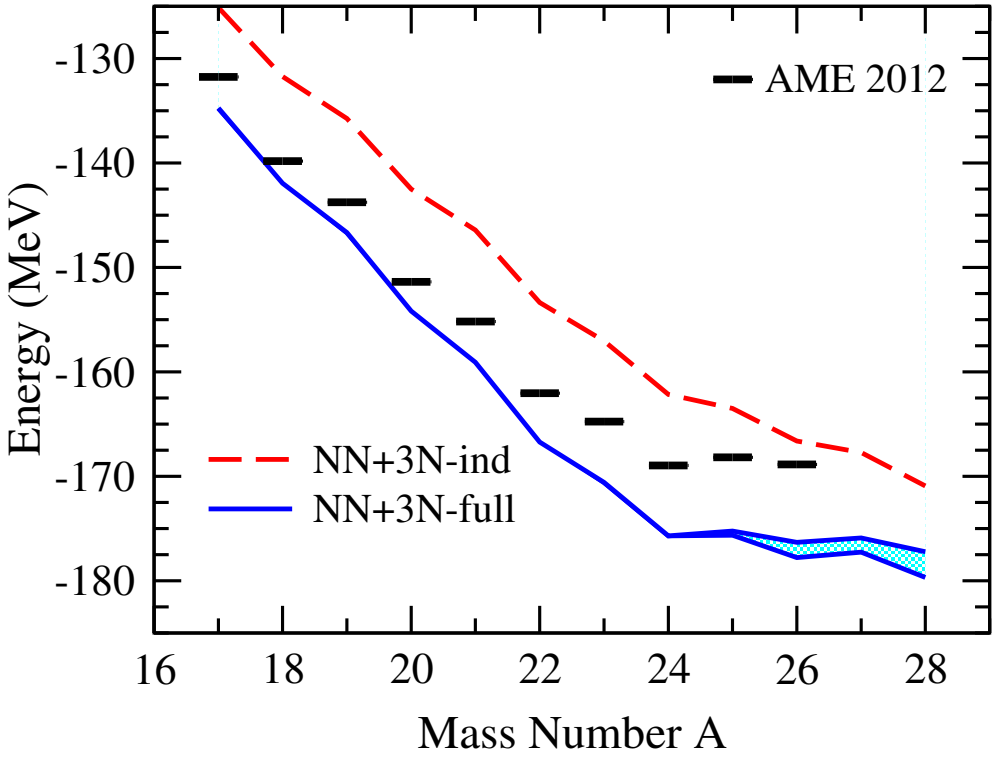


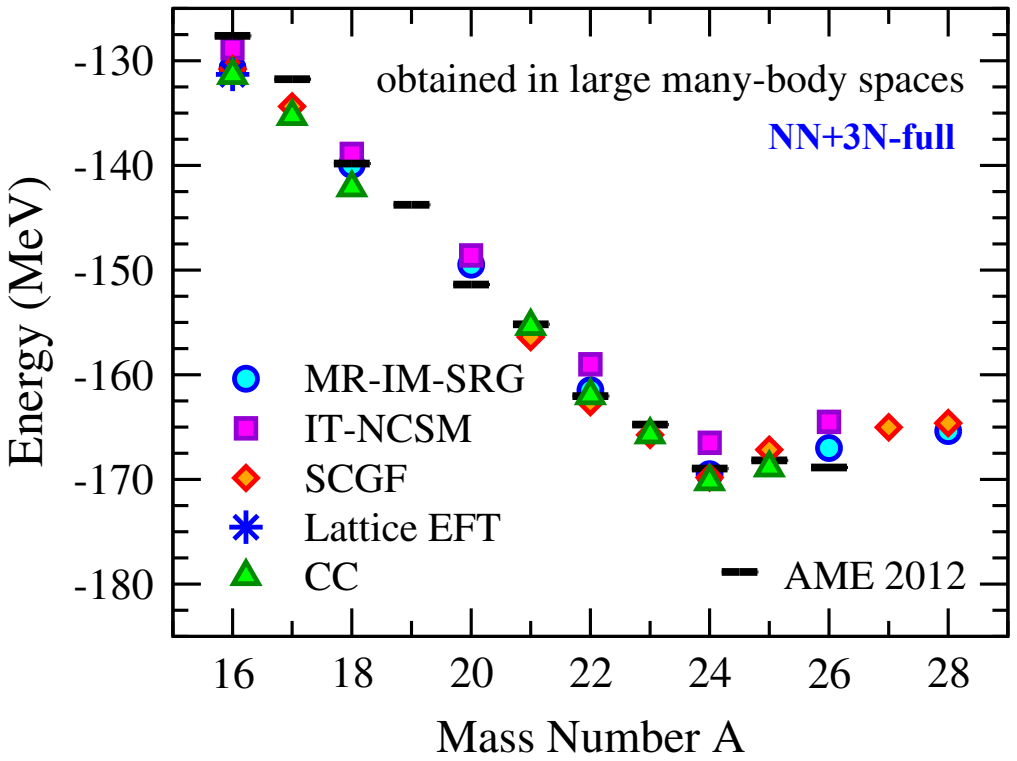
Agreement between all methods with same input forces

No reproduction of oxygen dripline in any case

Ground-State Energies in Oxygen Isotopes

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





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

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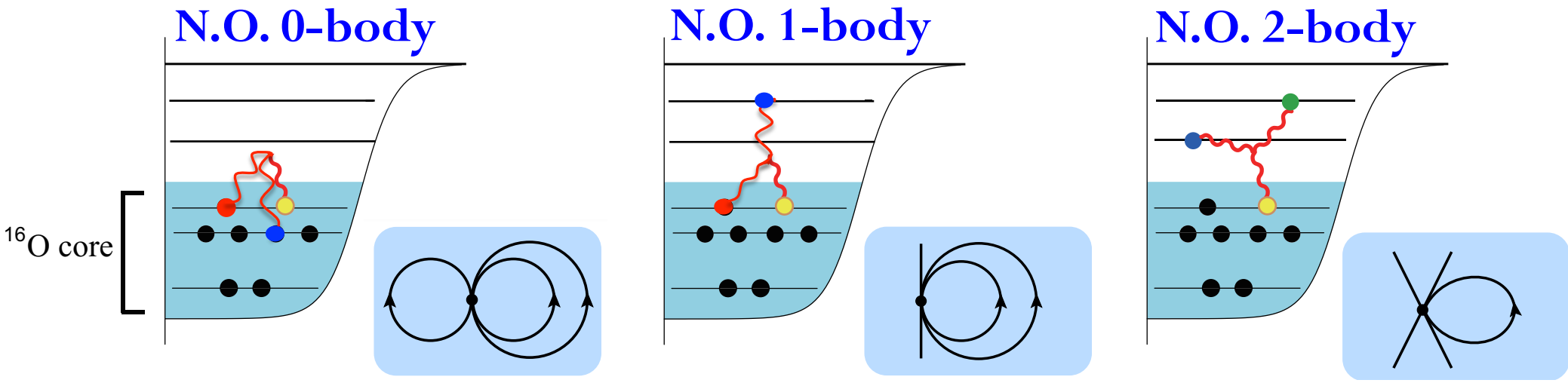
Clear improvement with NN+3N-full

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 nucleons

3N Forces in Valence Space

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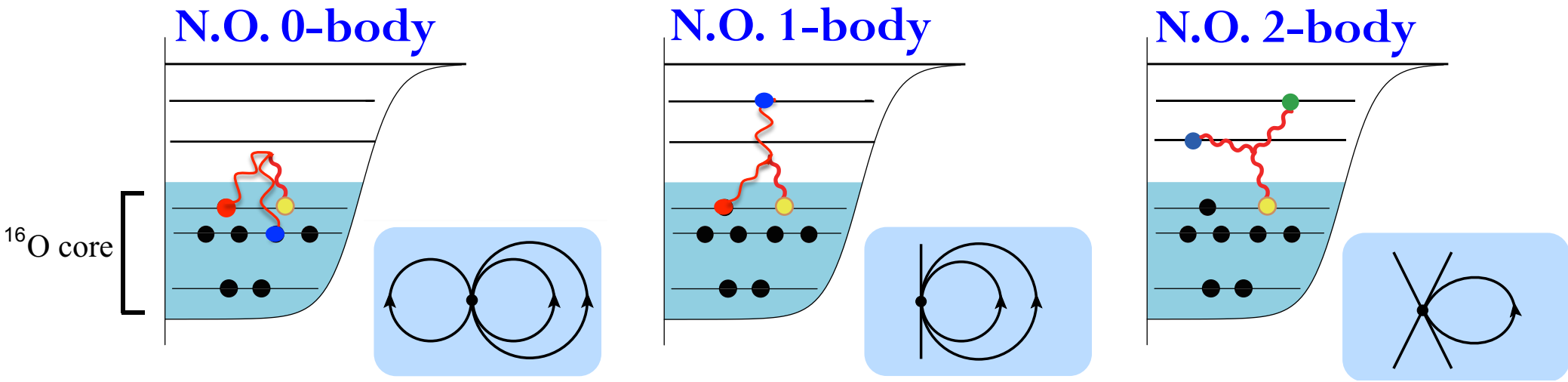
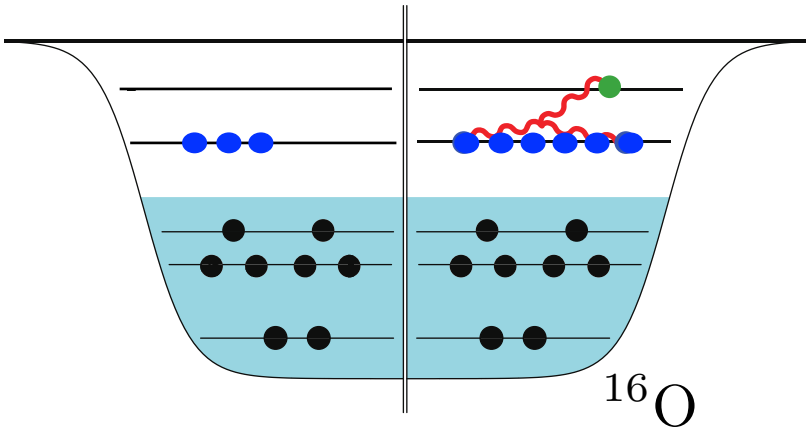
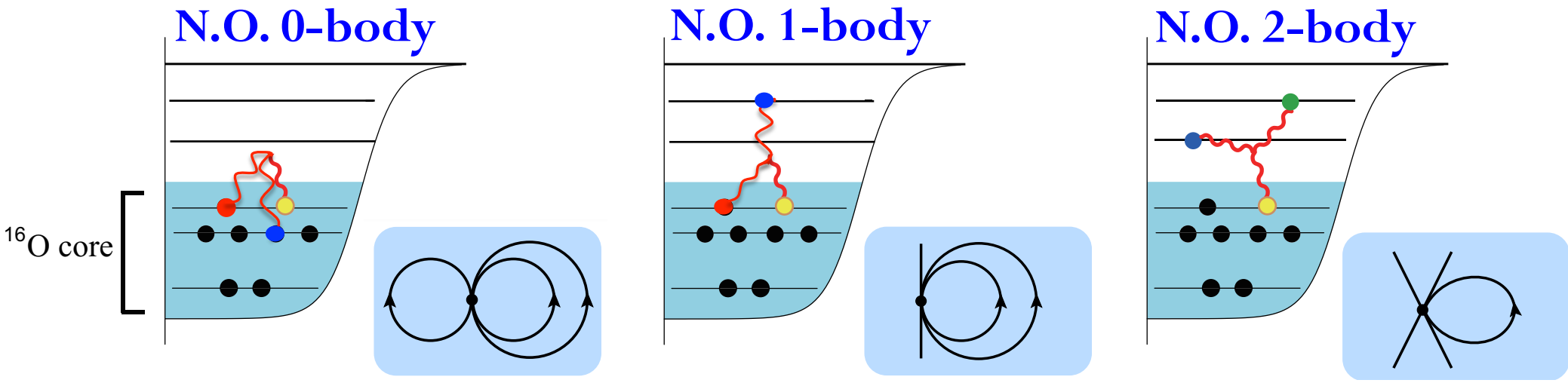


Neglect 3N forces between valence nucleons – significant as $N_v \sim N_c$



Targeted Normal Ordering

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



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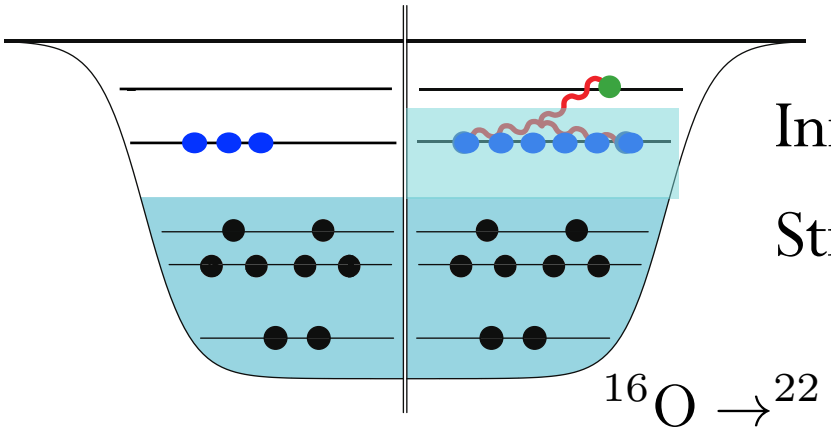
Capture these effects with new **Targeted N.O.**



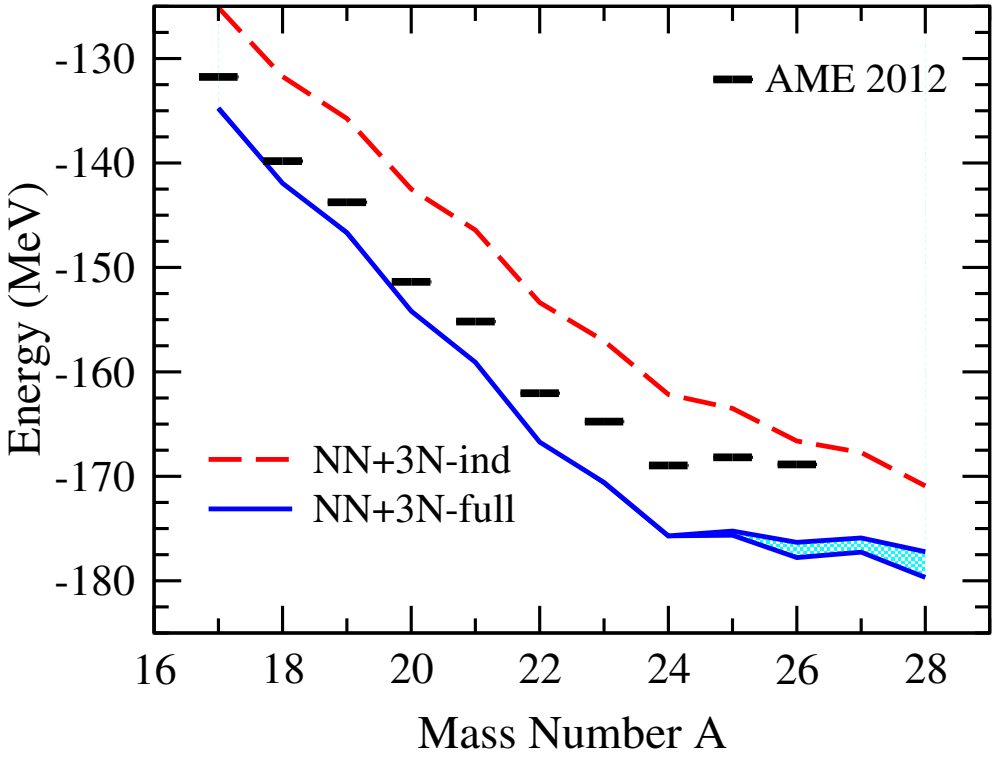
$^{16}\mathrm{O} \rightarrow {}^{22}\mathrm{O}$

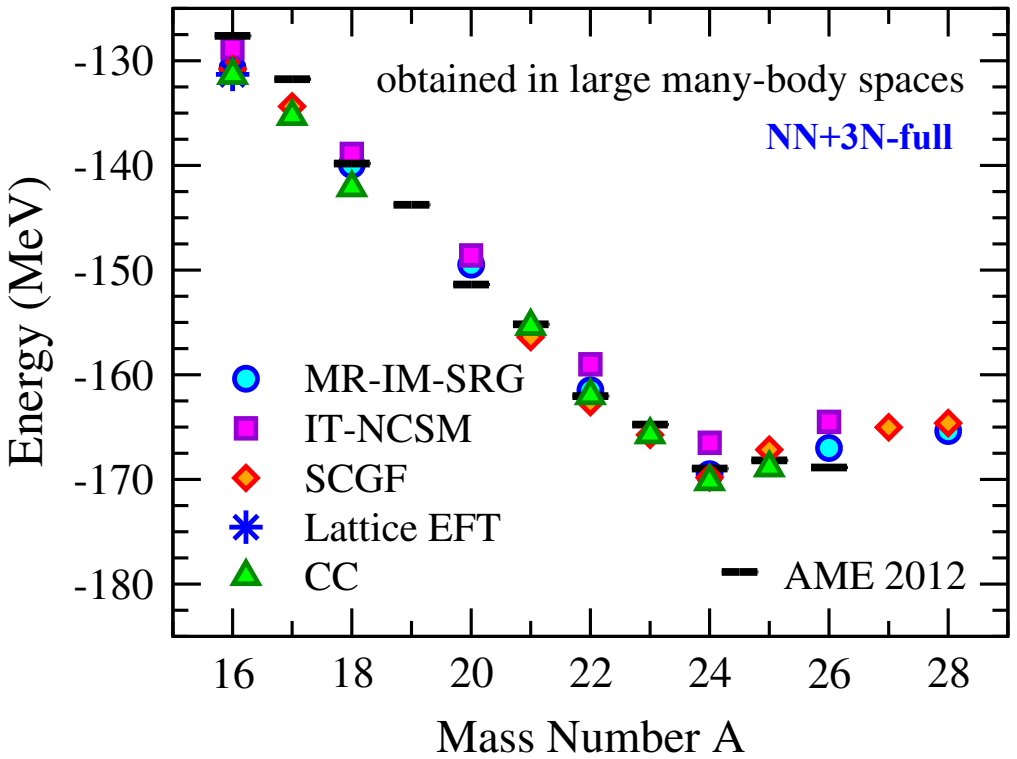
Initial N.O. wrt **nearest closed shell**

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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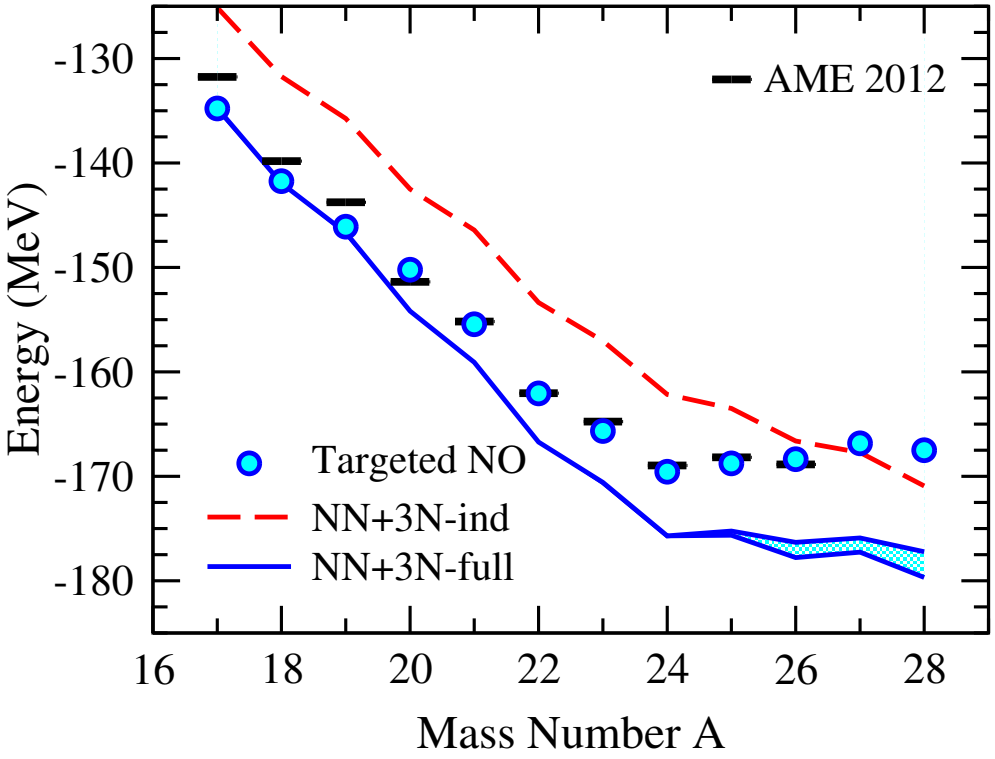
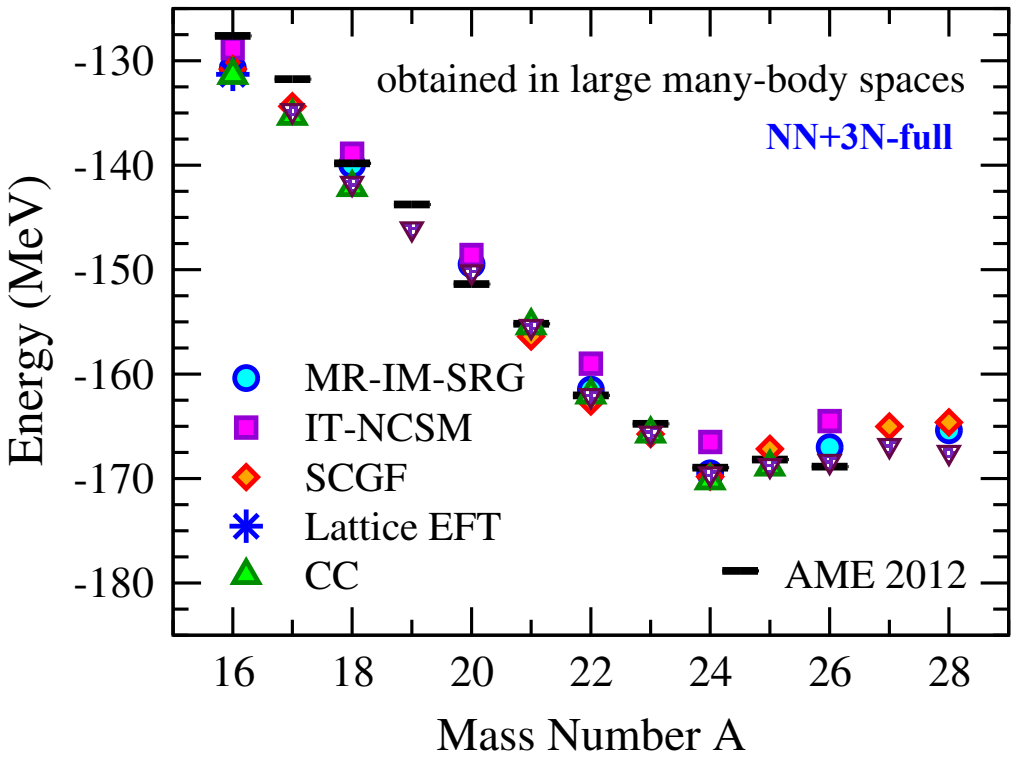




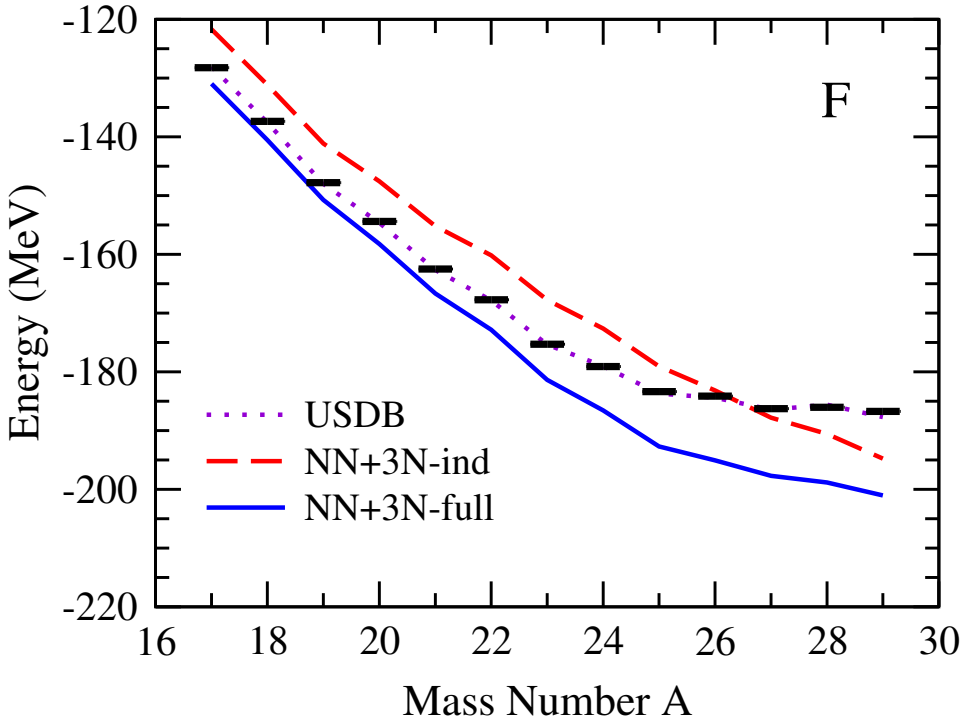
Hebeler, JDH, Menéndez, Schwenk, ARNPS (2015)

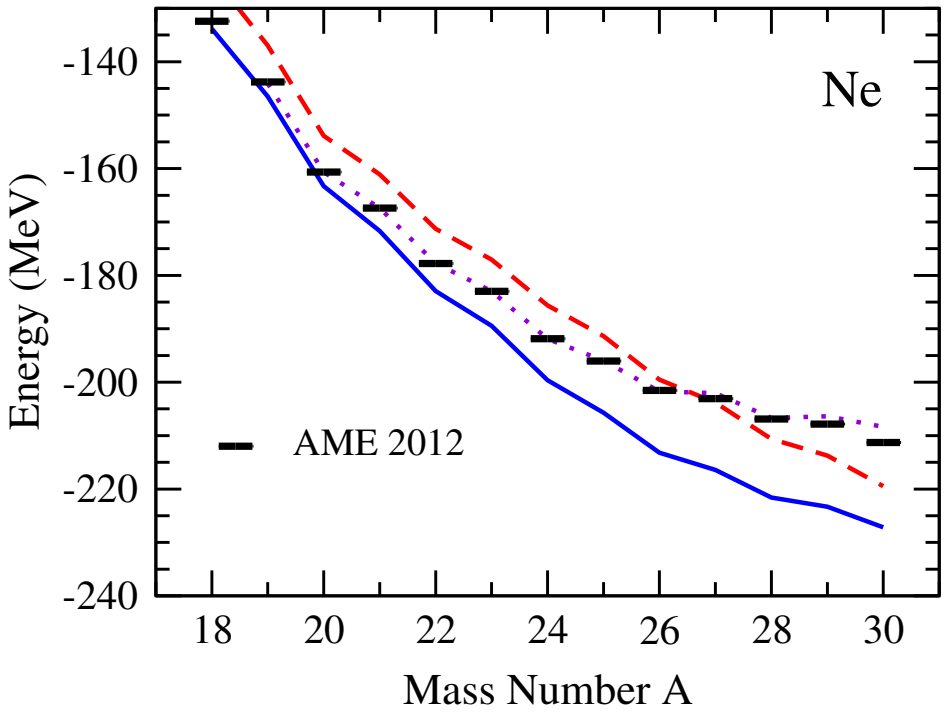
Improved method to capture neglected 3N forces in valence space

"Targeted" N.O. 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

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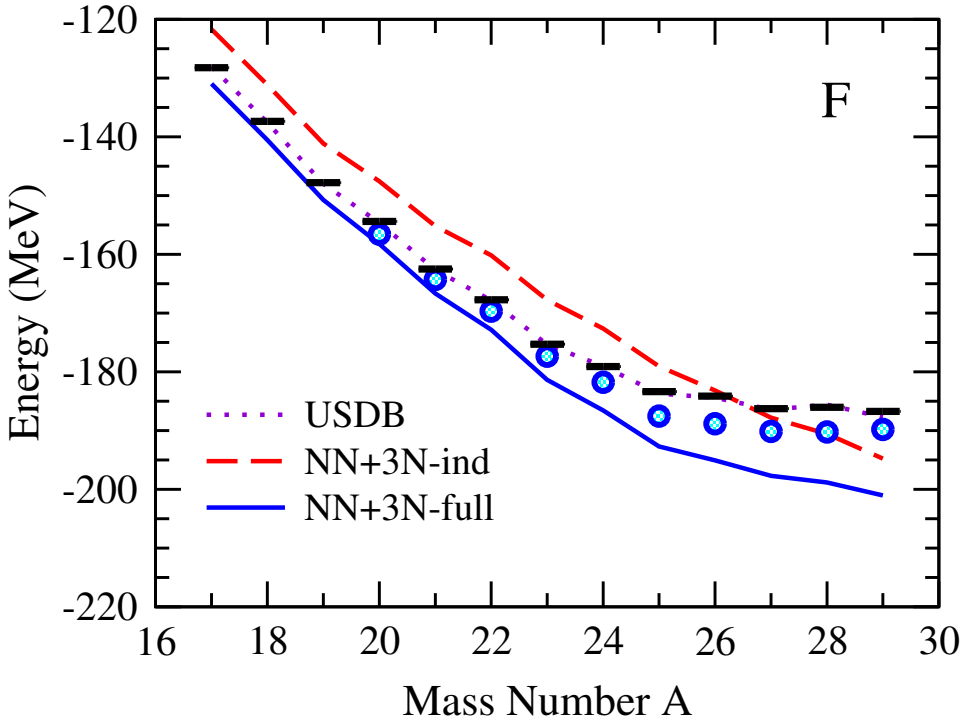

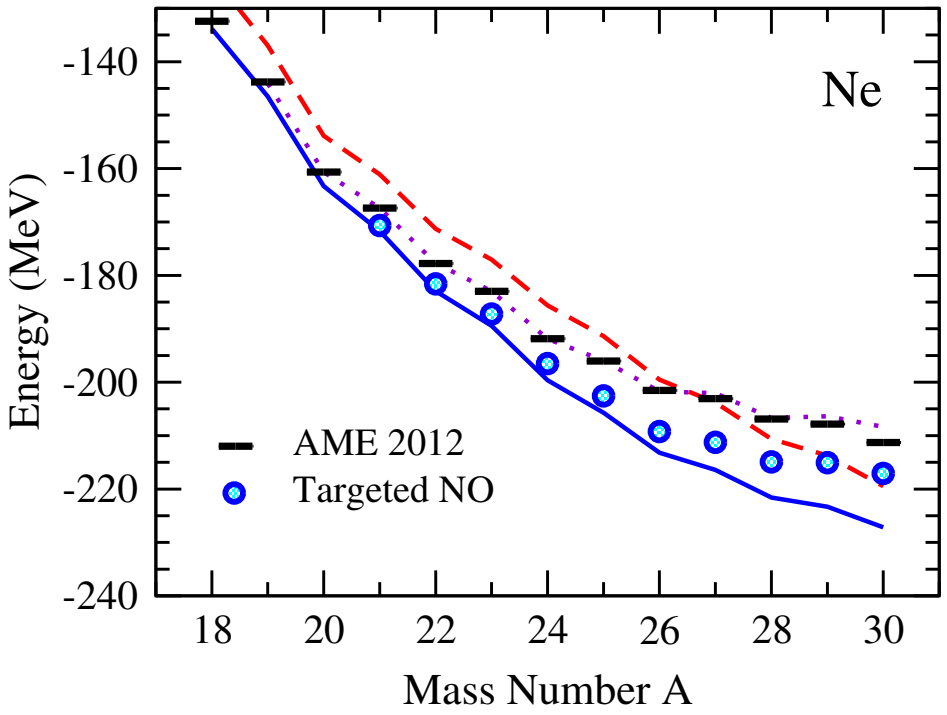

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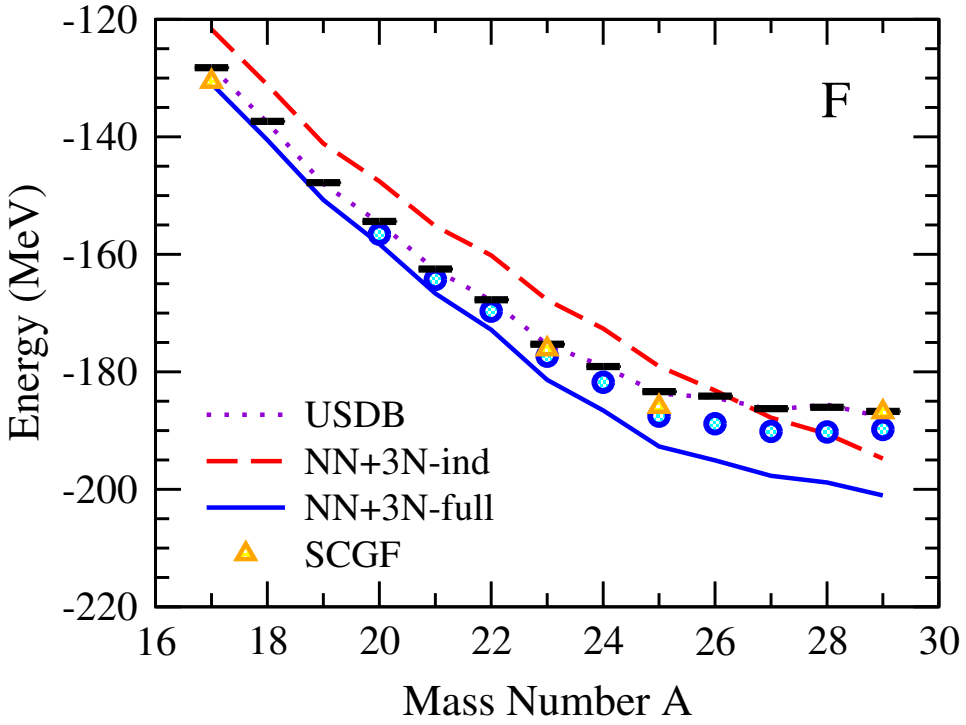

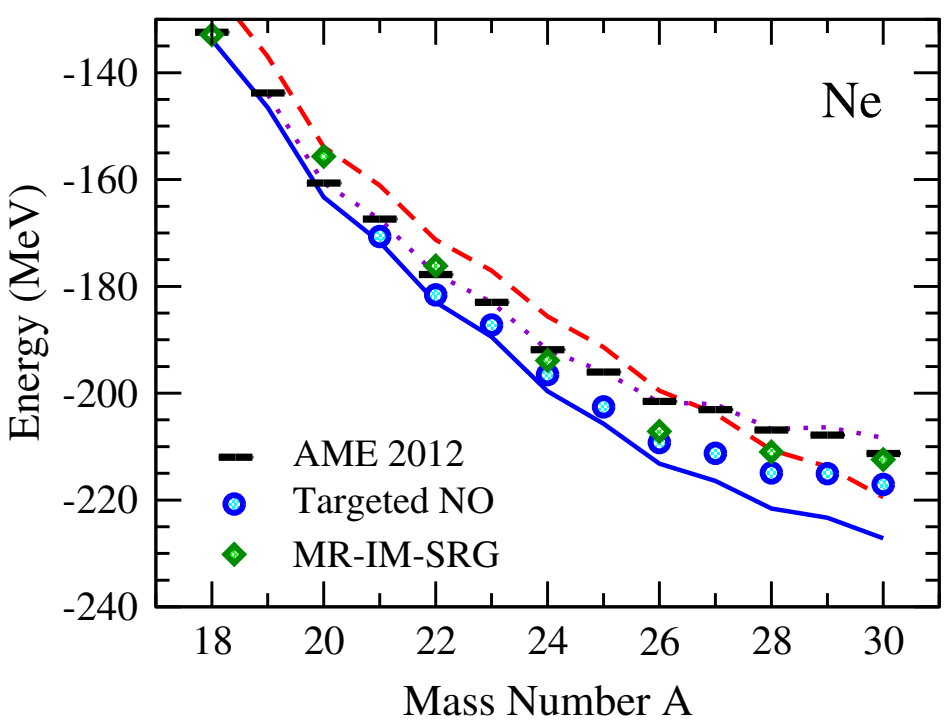

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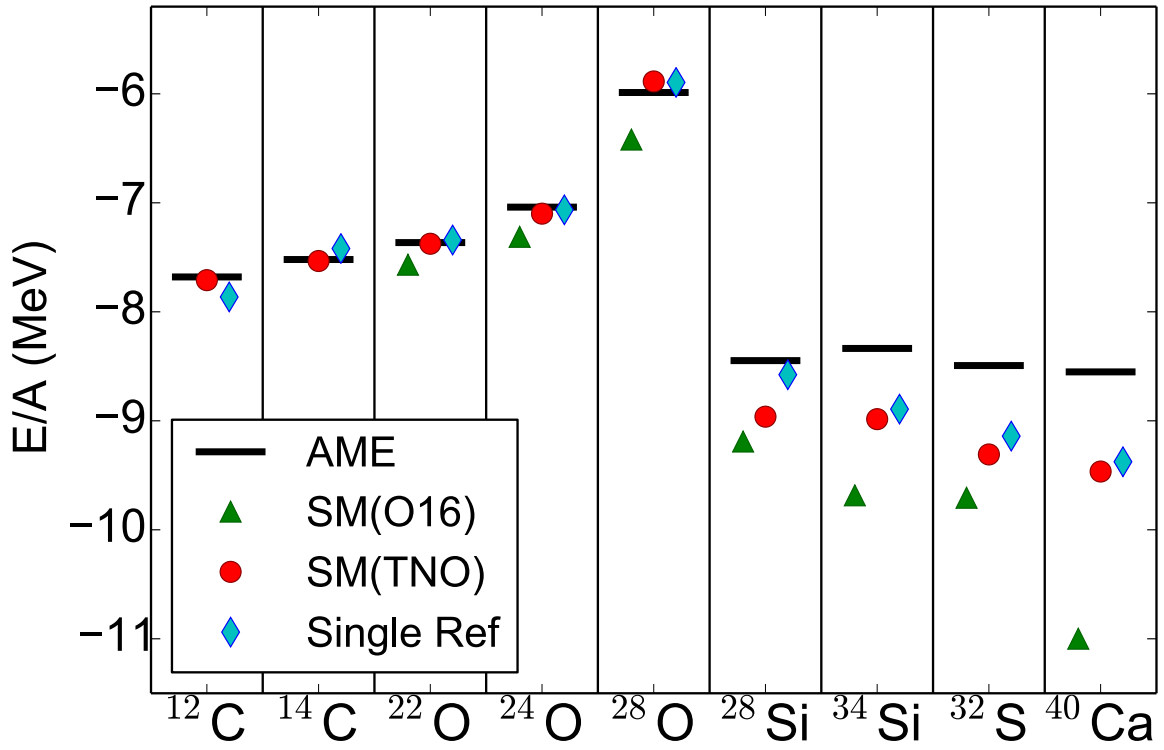
Good agreement with large-space ab initio SCGF and MR-IM-SRG!

Ground States from Oxygen to Calcium

3N force effects significant as N_v becomes large



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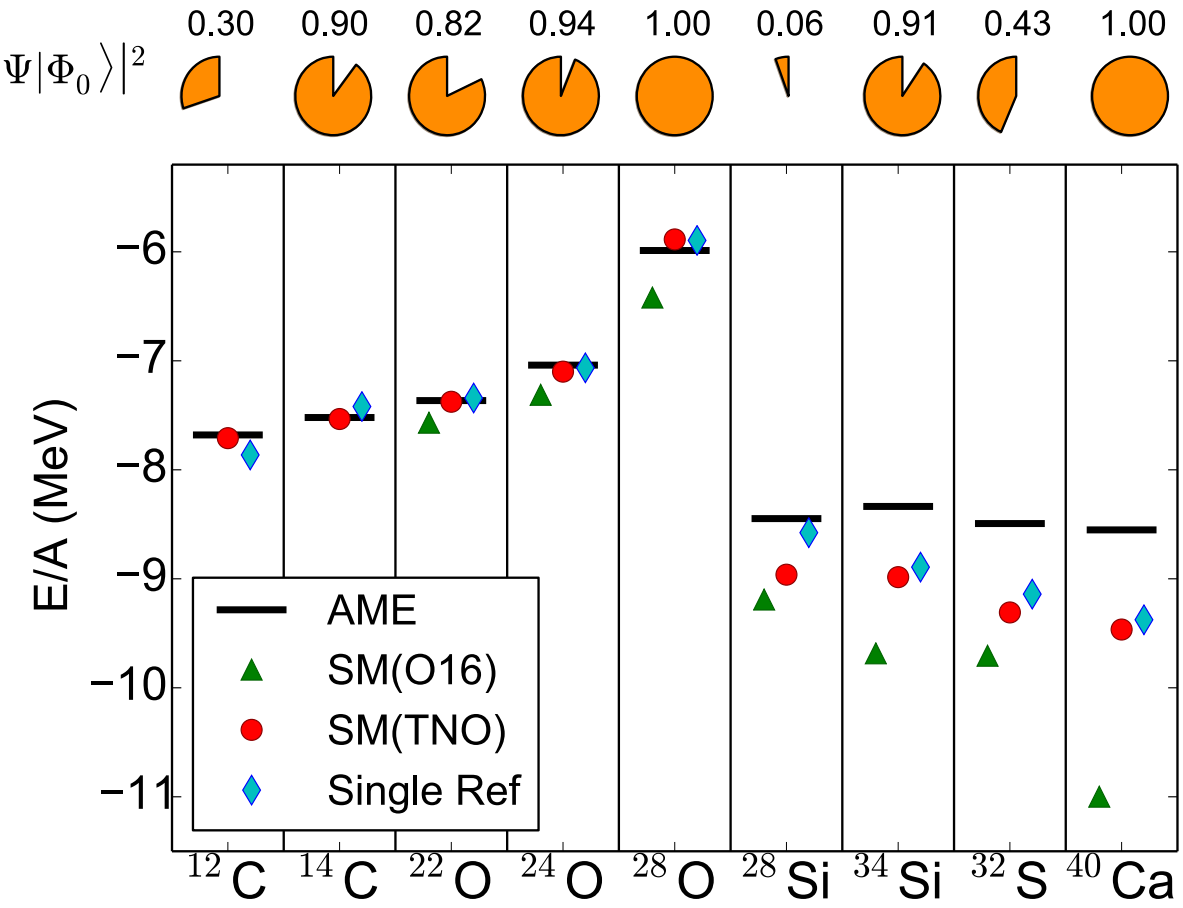

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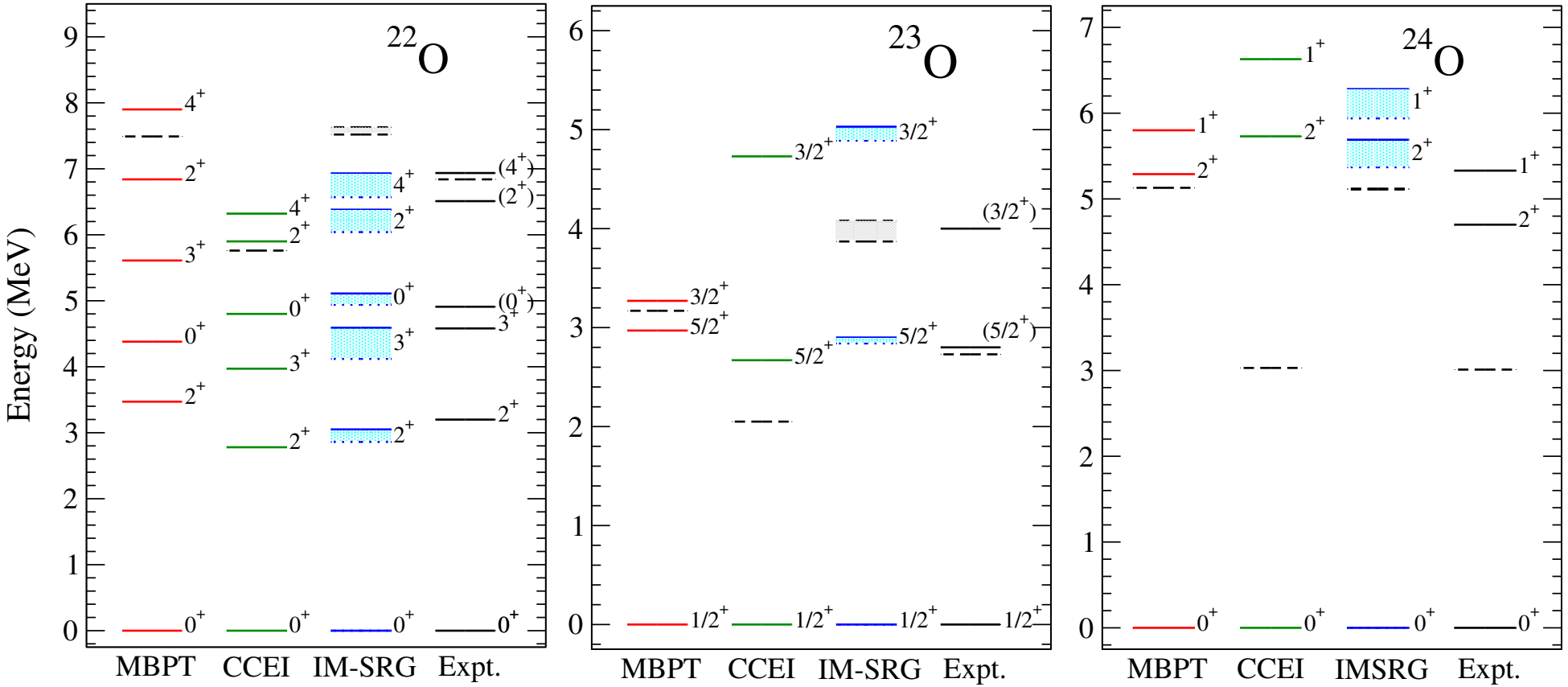
^{28}Si not good closed shell (single ref. calculation incorrect)

Discrepancy with experiment from initial nuclear interactions

Comparison with MBPT/CCEI Oxygen Spectra

Neutron-rich oxygen spectra from existing shell-model approaches



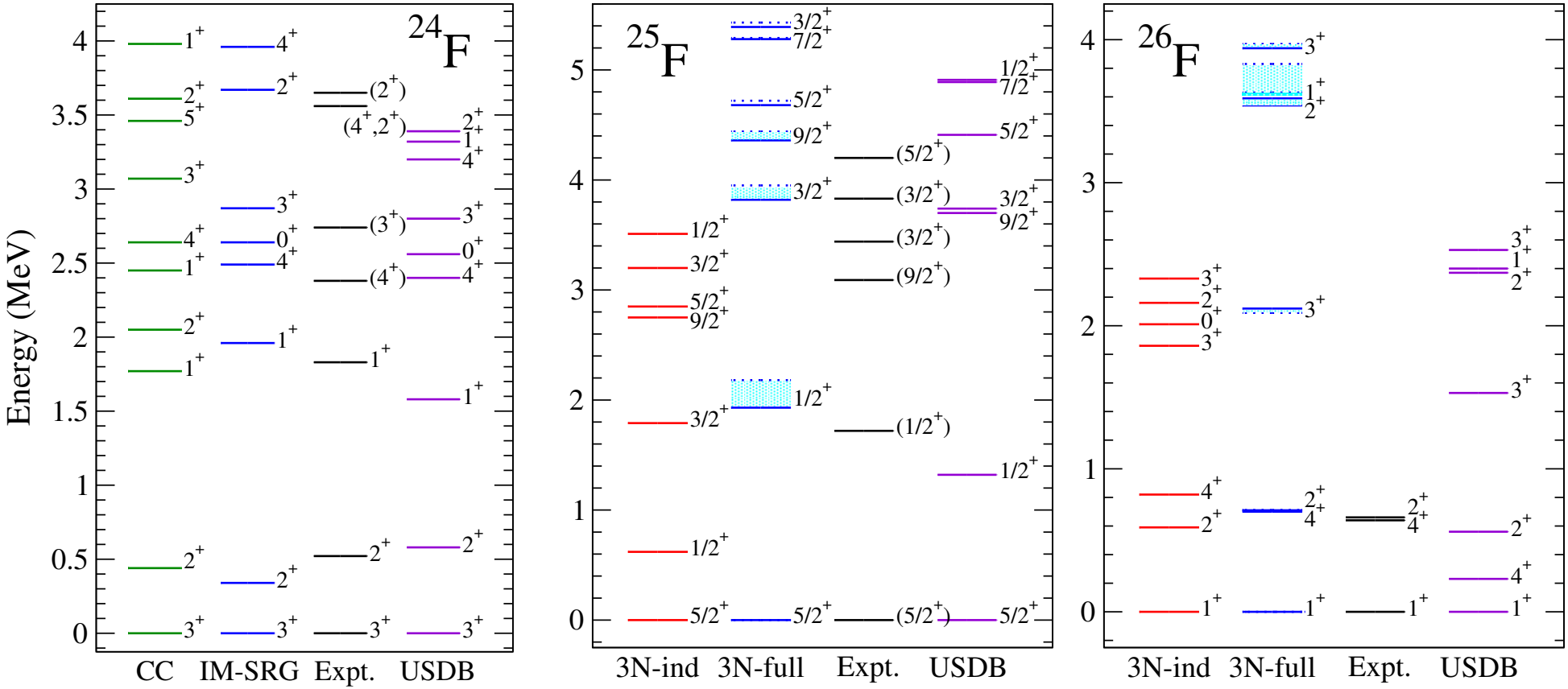
Hebeler, JDH, Menéndez, Schwenk, ARNPS (2015)

MBPT in extended valence space

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

Doubly Open Shell: Neutron-Rich F Spectra

Fluorine spectroscopy: **NN+3N-ind** and **NN+3N-full**, **Full CC**



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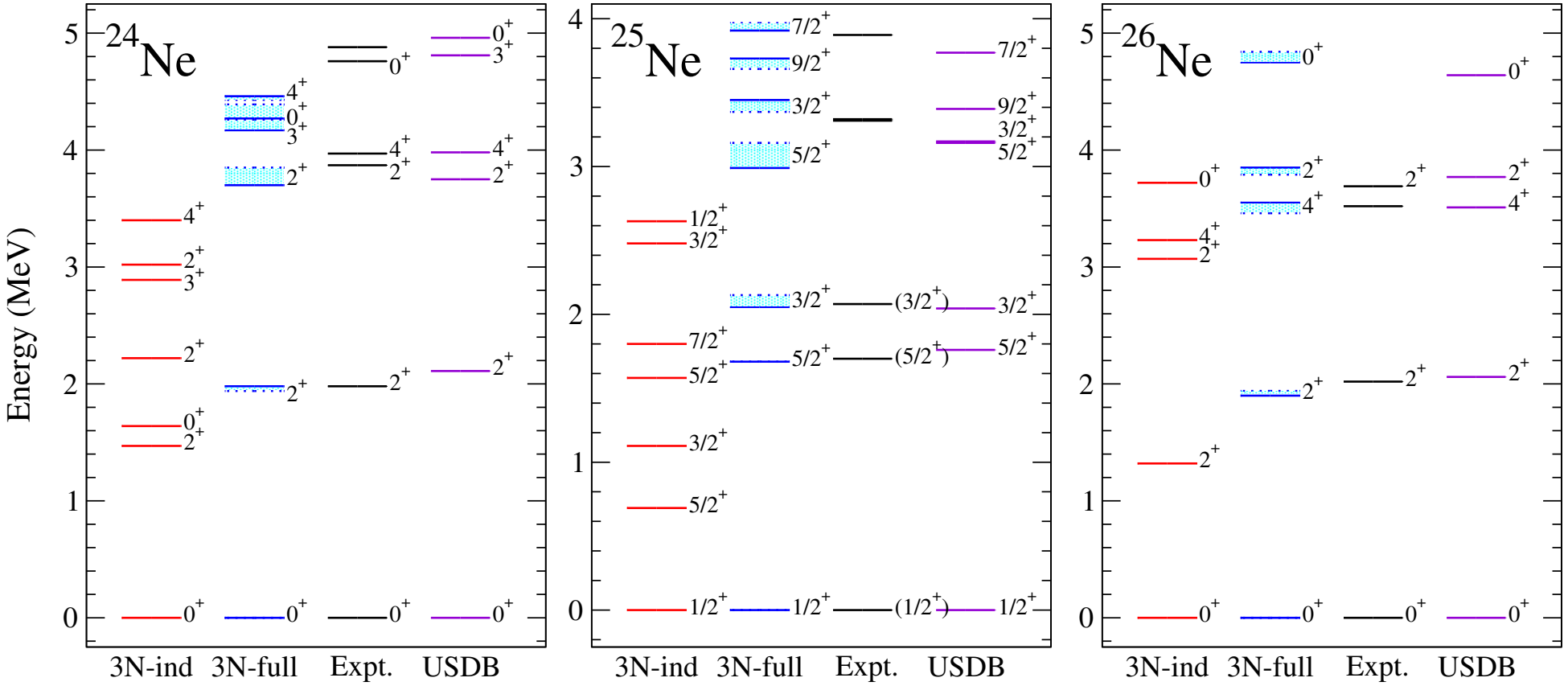
IM-SRG: **competitive with phenomenology**, good agreement with data

Doubly Open Shell: Neutron-Rich Ne Spectra

Neon spectroscopy: **NN+3N-ind** and **NN+3N-full**



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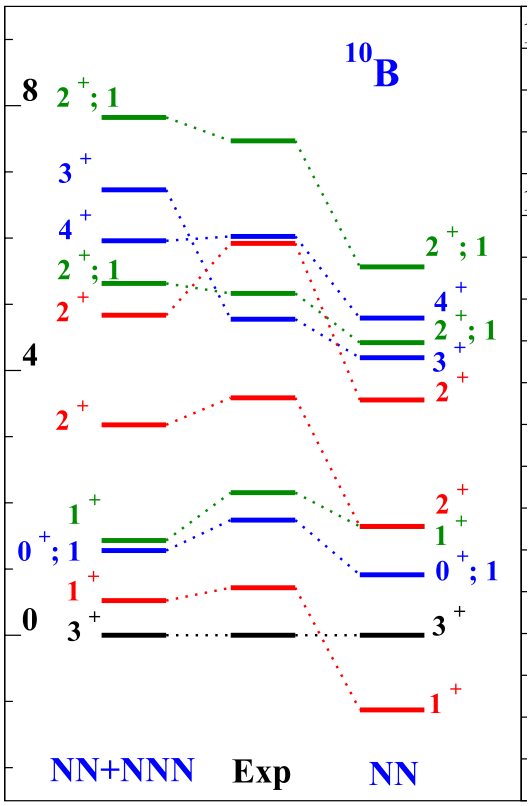
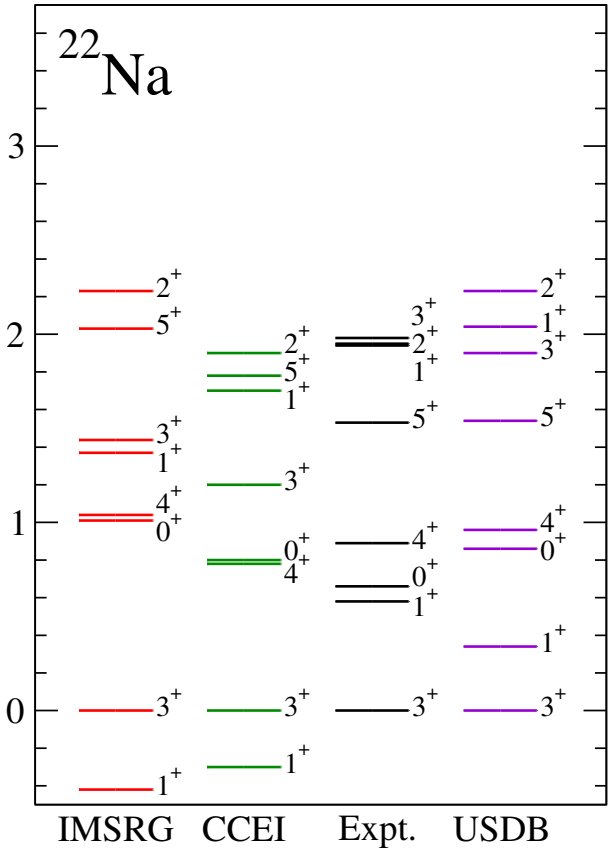
The Special Case of ^{22}Na

Without 3N forces same $1^+ - 3^+$ inversion as the famous case in ^{10}B



Navratil et al., PRL (2007)

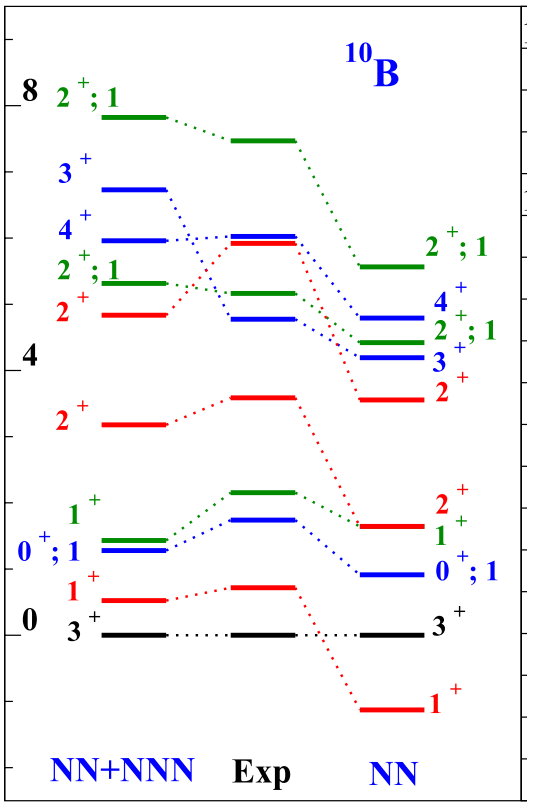


Stroberg et al., arXiv:1511.03802

With 3N forces IM-SRG, CCEI both predict incorrect 1^+ ground state

The Special Case of ^{22}Na

Without 3N forces same $1^+ - 3^+$ inversion as the famous case in ^{10}B



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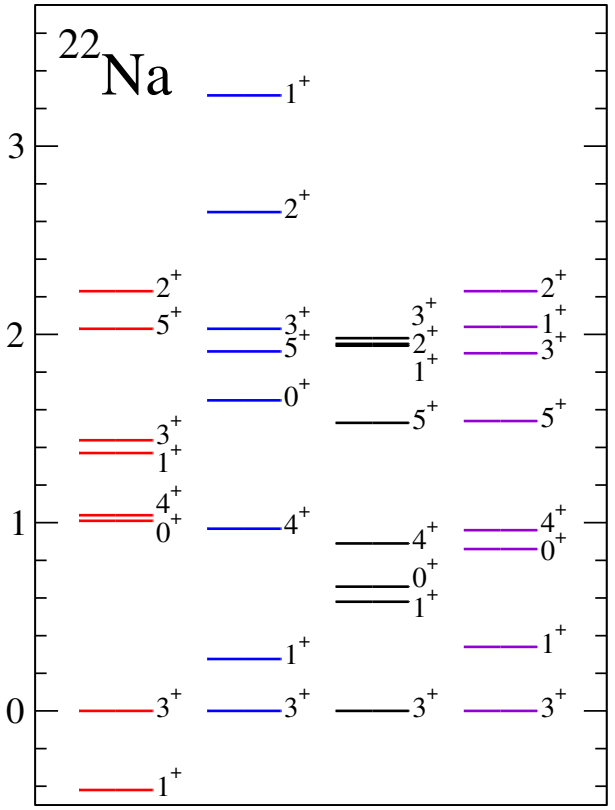


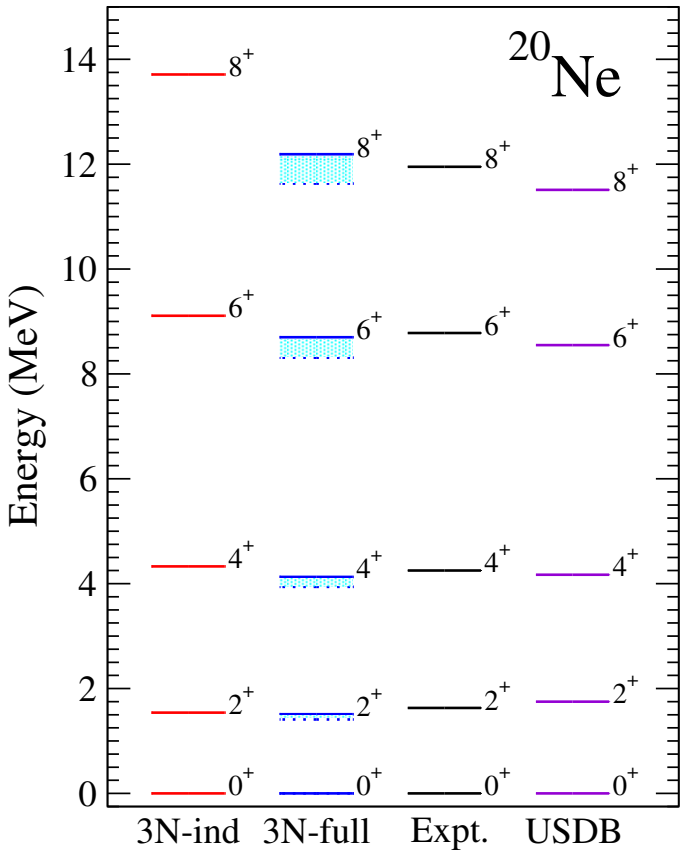
Stroberg et al., arXiv:1511.03802

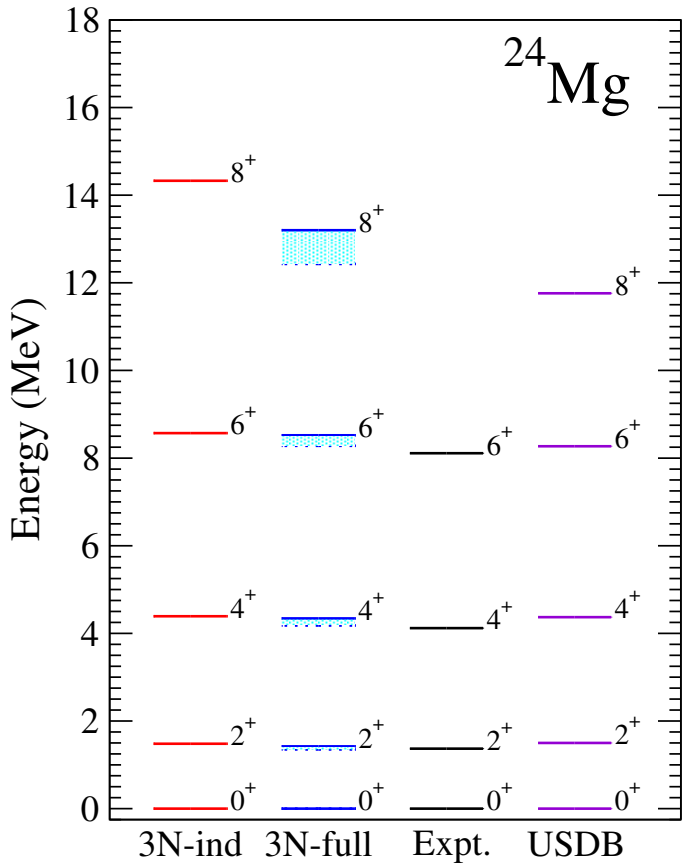
With 3N forces IM-SRG, CCEI both predict incorrect 1^+ ground state

With ^{28}Si reference for TNO, correct 3^+ ground state predicted

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

Ground-state rotational band for well-known deformed nuclei





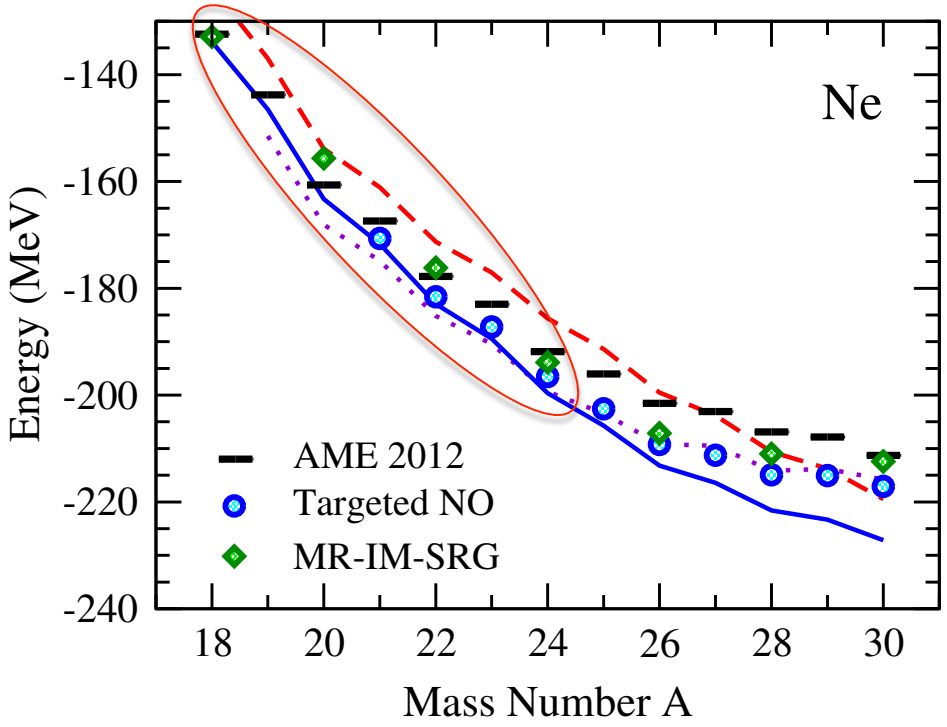
Stroberg et al., arXiv:1511.03802

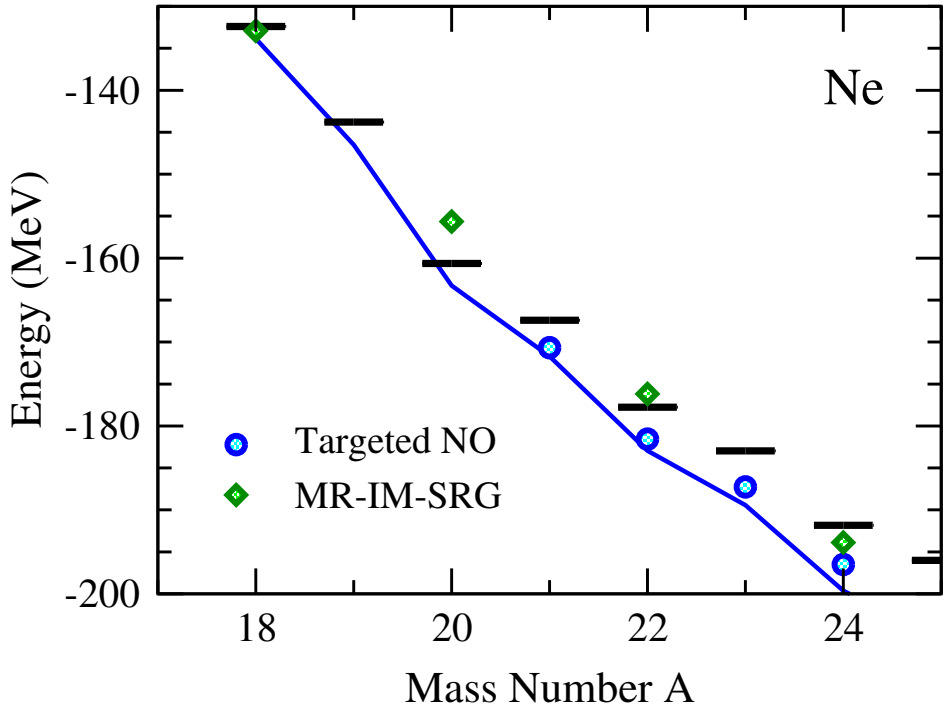
IM-SRG: **competitive with phenomenology**, good agreement with data

First description of deformation from ab initio methods (trivial in shell model)

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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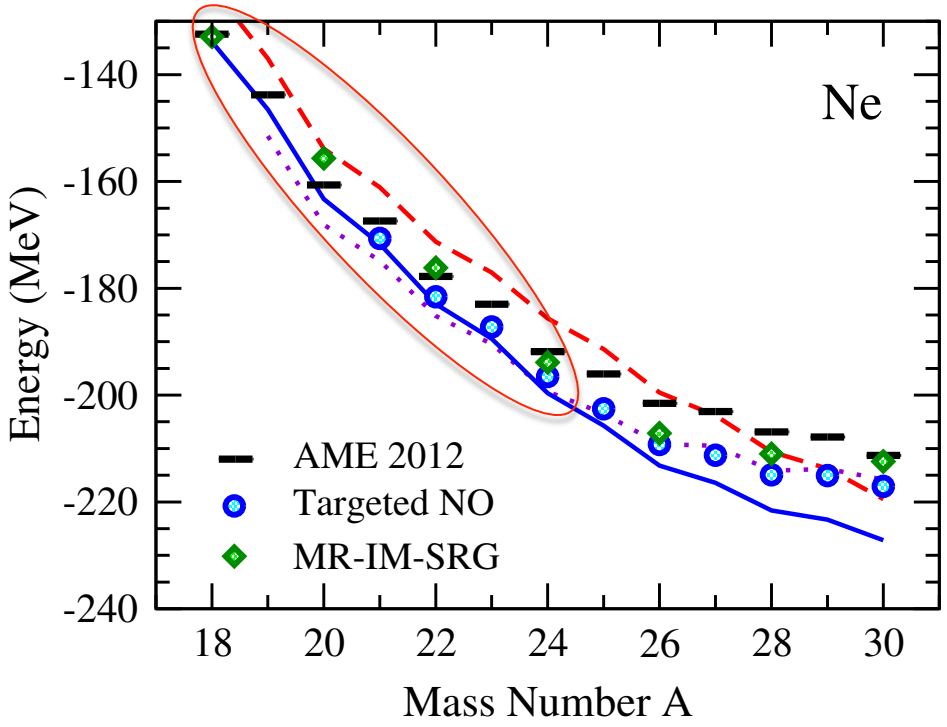
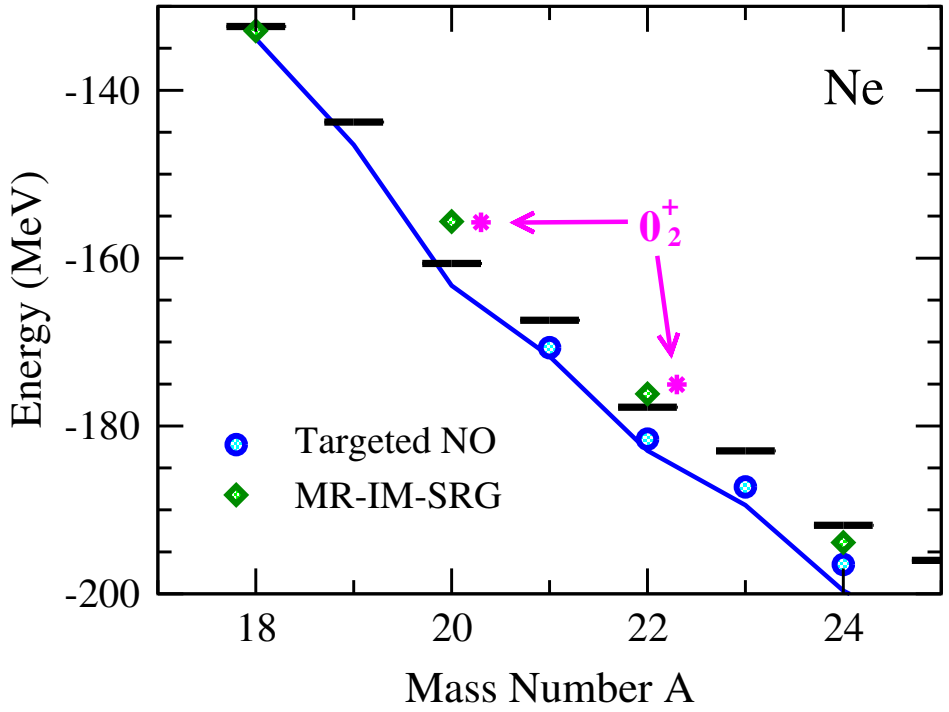




MR-IM-SRG built on spherical reference state

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

New Approach: Magnus Expansion

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

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

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

Solve flow equation for:

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

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

Ab Initio Effective Valence-Space Operators

Keep unitary transformation from evolution of Hamiltonian

Can generalize to arbitrary operators:

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

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

Requires normal-ordered operators in *J*-coupled basis

First application to scalar operators (radii, E0) straightforward

Scalar Operators: E0 Transitions and Radii

Seldom calculated in nuclear shell model

In single HO shell:

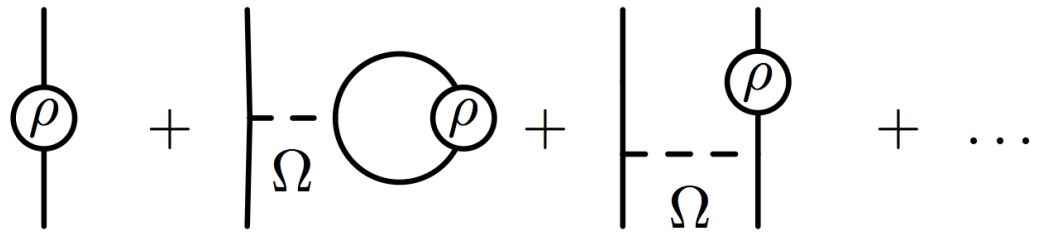
$$|\langle f|\rho_{E0}|i\rangle|^2 \propto \delta_{ij} \text{ where } \rho_{E0} = \frac{1}{e^2 R}\sum_i e_i r_i^2$$

Must resort to 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



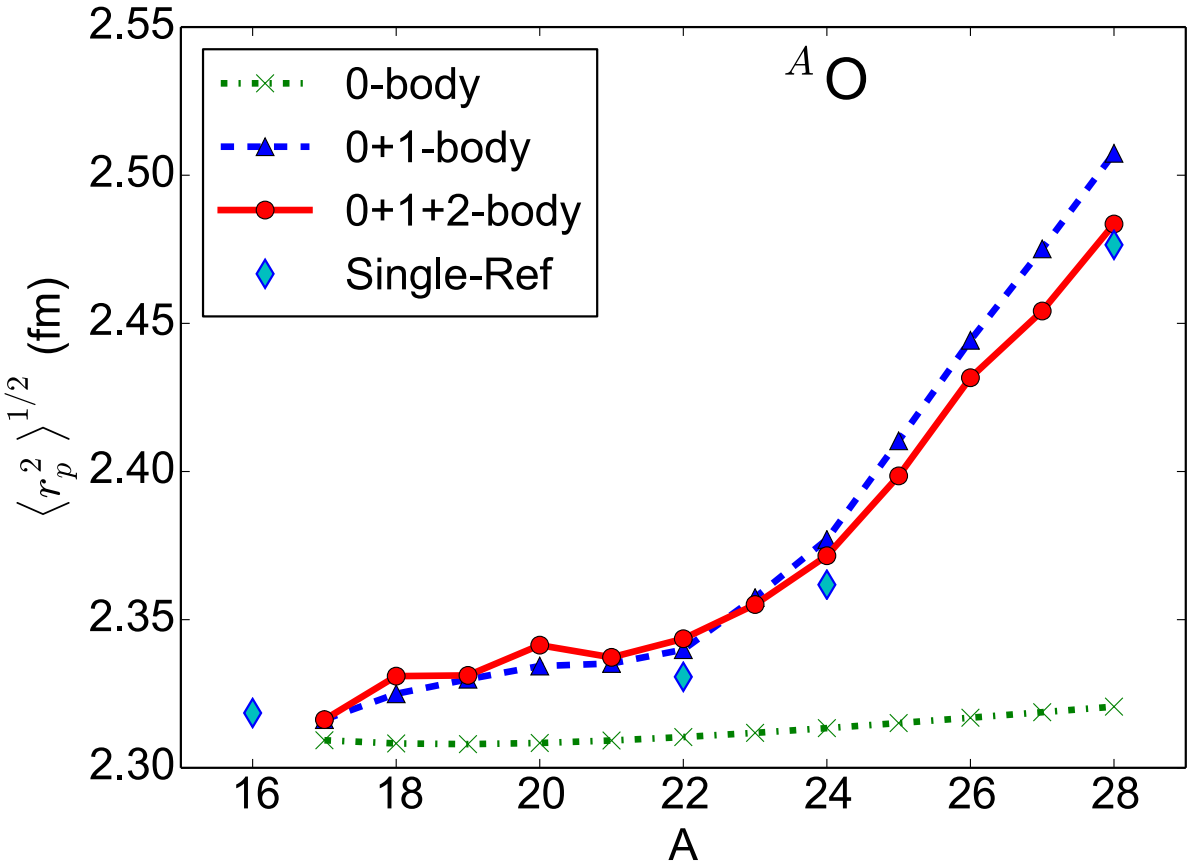
Quantify importance of induced higher-body contributions

RMS Point Proton Radii in Oxygen

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

$$\tilde{R}^2 = U R^2 U^\dagger \qquad \left\langle R^2 \right\rangle = \left\langle \Phi_0 \mid \tilde{R}^2 \mid \Phi_0 \right\rangle + \left\langle \Phi_{\rm SM} \mid \tilde{R}^2 \mid \Phi_{\rm SM} \right\rangle$$

Calculate absolute radii for all sd-shell nuclei



Stroberg et al., in prep

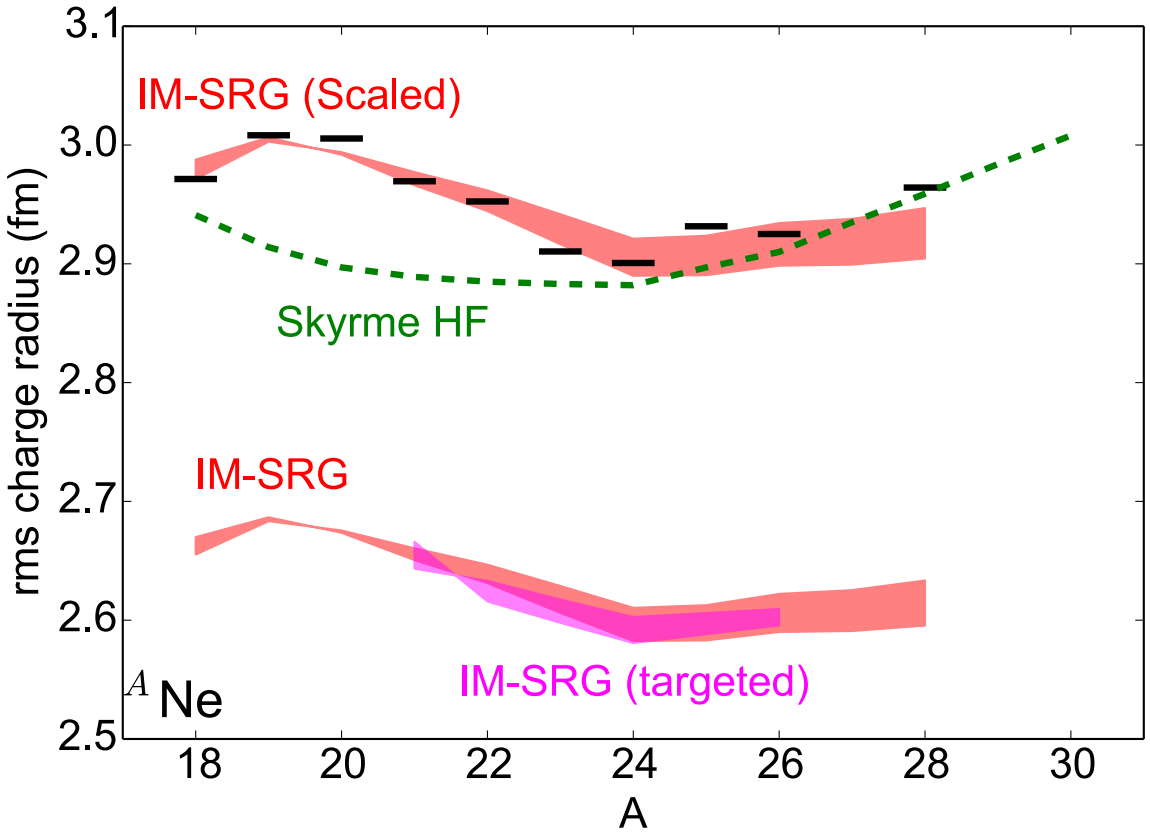
Full shell model tracks large-space single-reference IMSRG results

RMS Charge Radii in Neon

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

$$\tilde{R}^2 = U R^2 U^\dagger \qquad \langle R^2 \rangle = \left\langle \Phi_0 \mid \tilde{R}^2 \mid \Phi_0 \right\rangle + \left\langle \Phi_{\rm SM} \mid \tilde{R}^2 \mid \Phi_{\rm SM} \right\rangle$$

Calculate absolute radii for full sd-shell



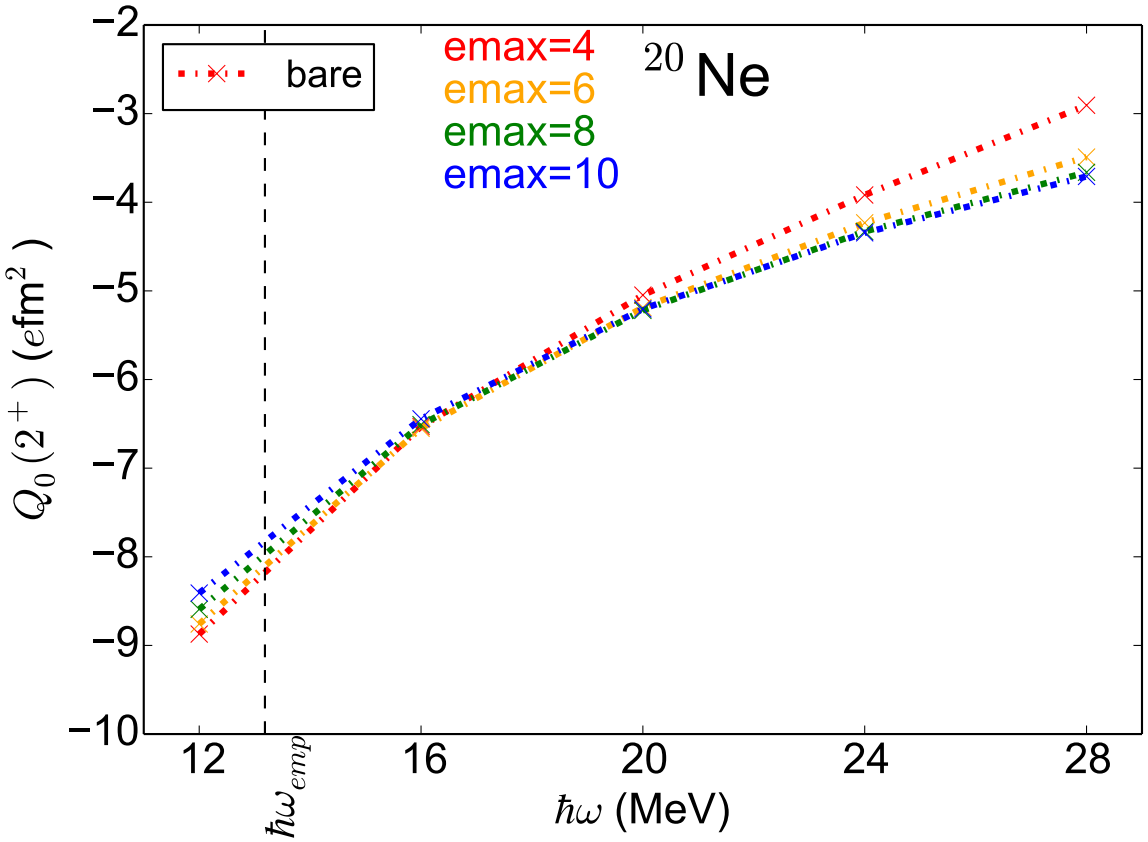
Stroberg et al., in prep

Initial Hamiltonian deficient – signature of deformation reproduced

Tensor Operators: Quadrupole Moments

First results for effective valence-space tensor operators

Convergence of quadrupole moments



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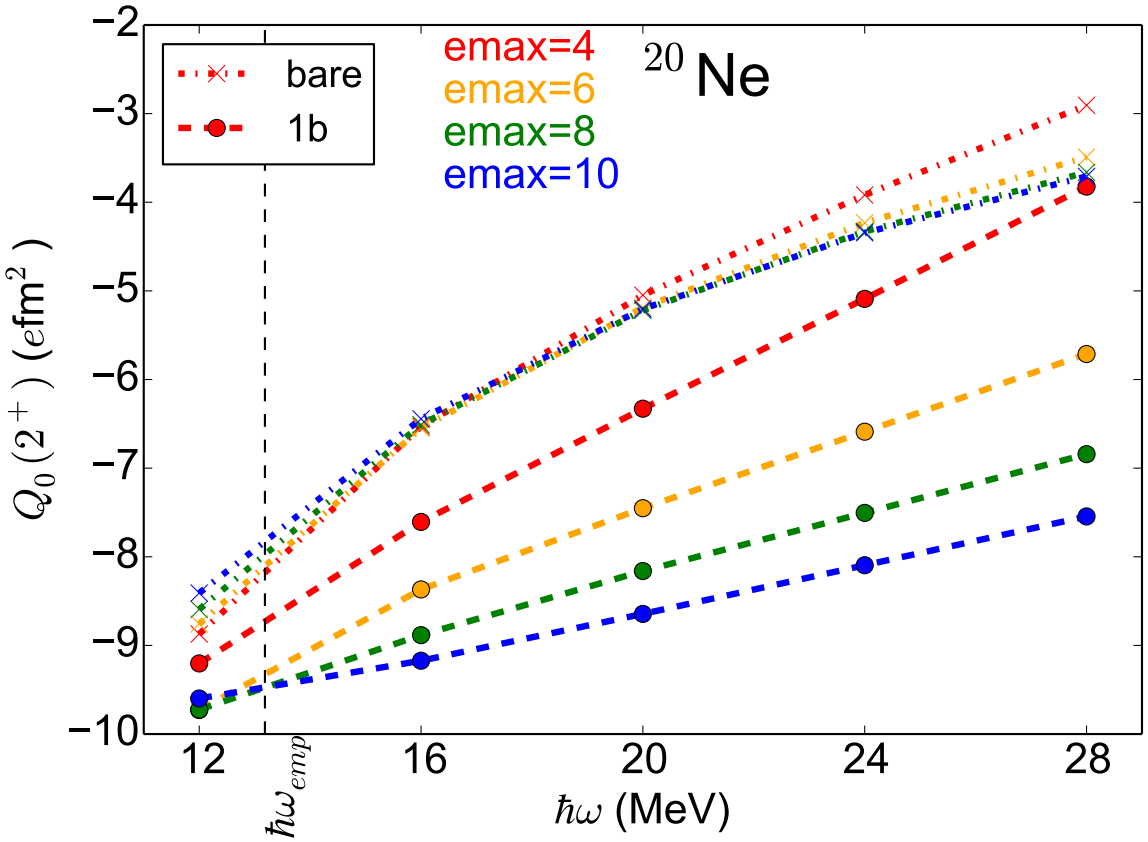

Large effect from renormalized 1-body part

emax=12,14 uderway

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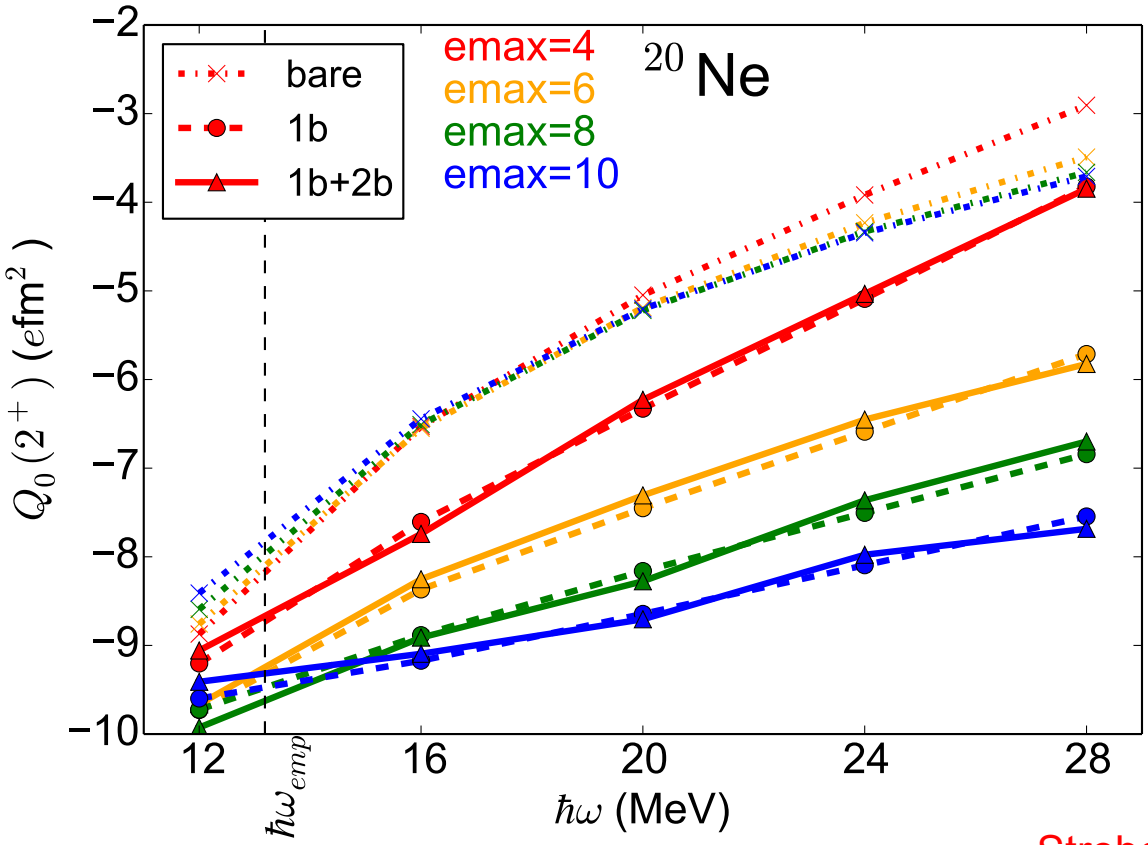

Stroberg et al., in prep

Largest effect from renormalized 1-body part, 2-body minimal change

emax=12,14 uderway

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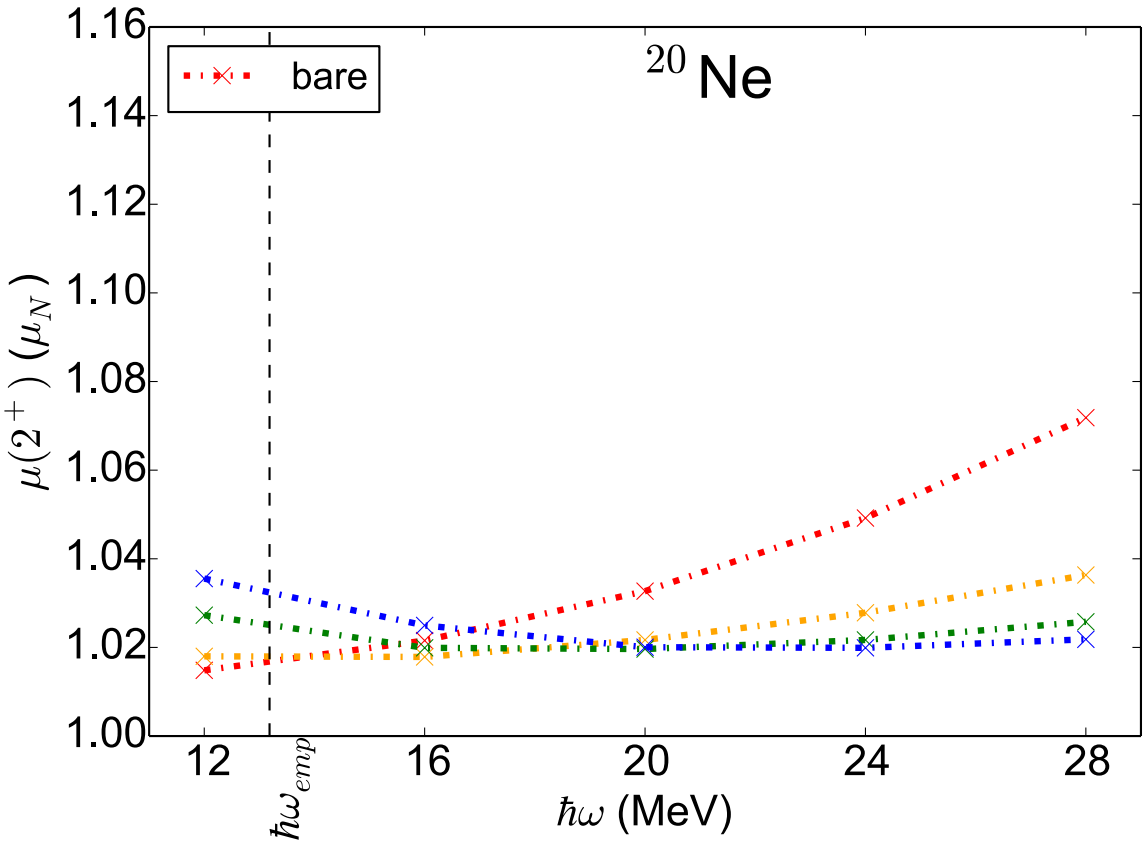

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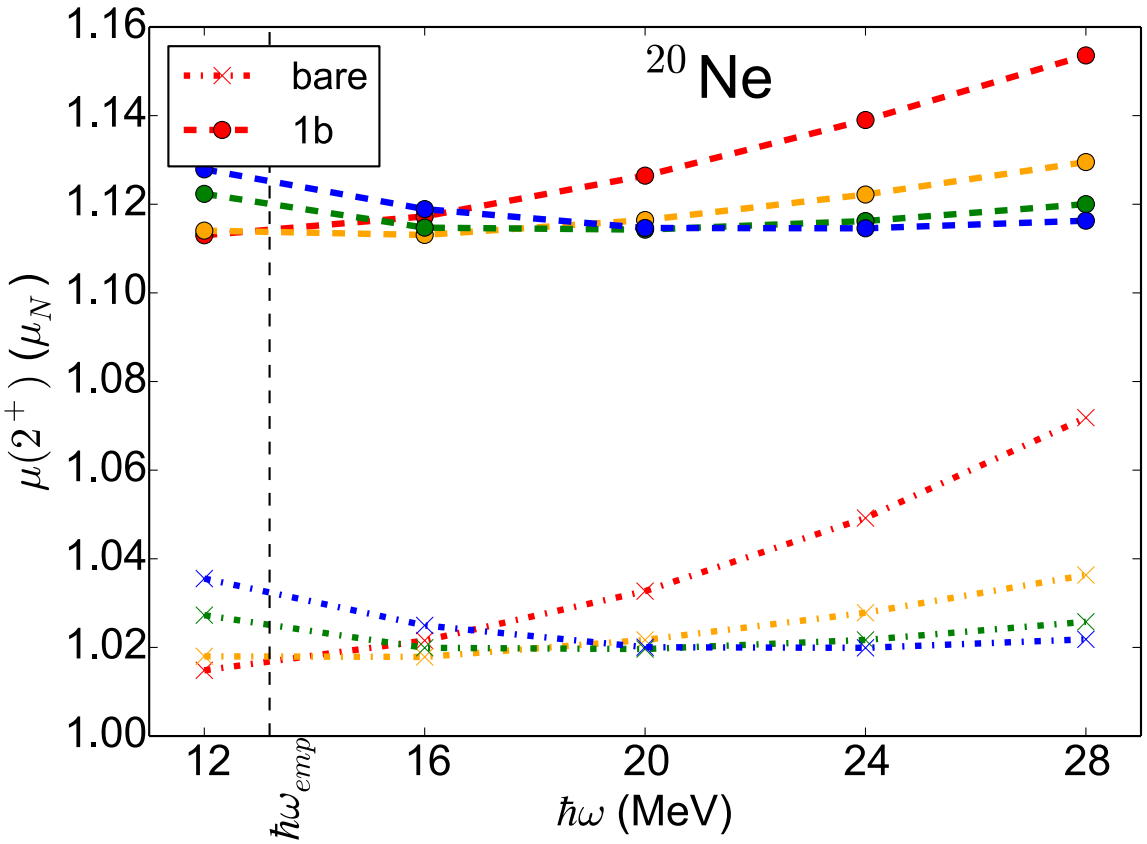

Renormalized 1-body gives significant effect

Tensor Operators: Magnetic Moments

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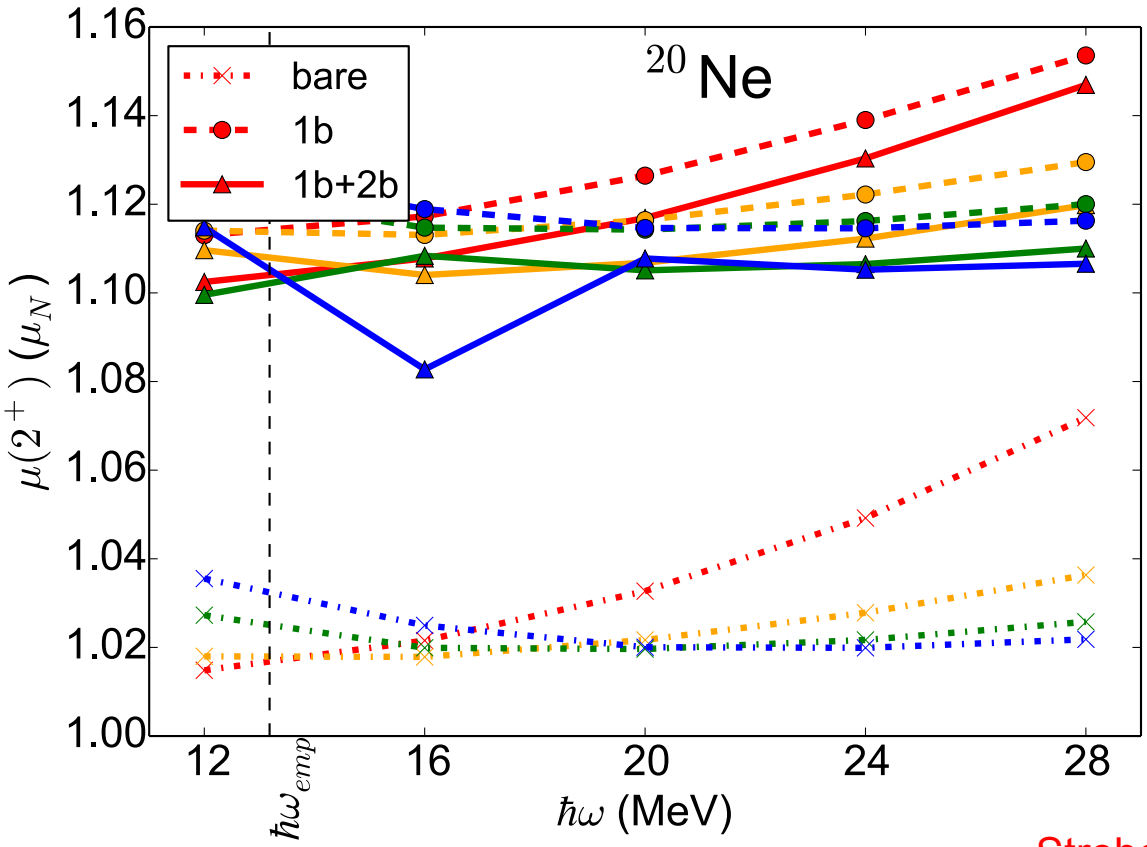


Stroberg et al., in prep

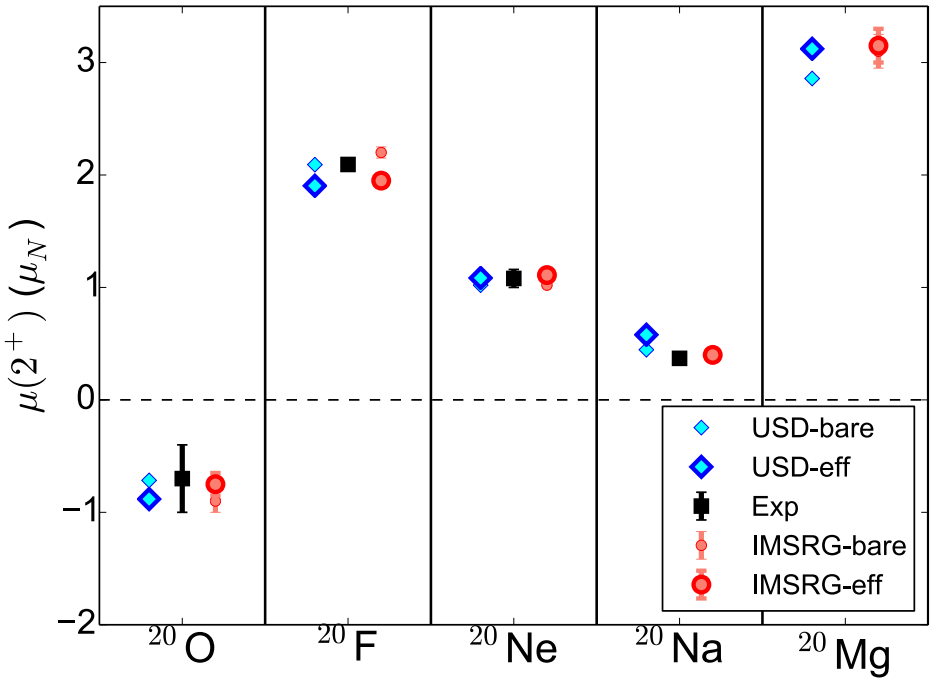
Renormalized 1-body gives significant effect

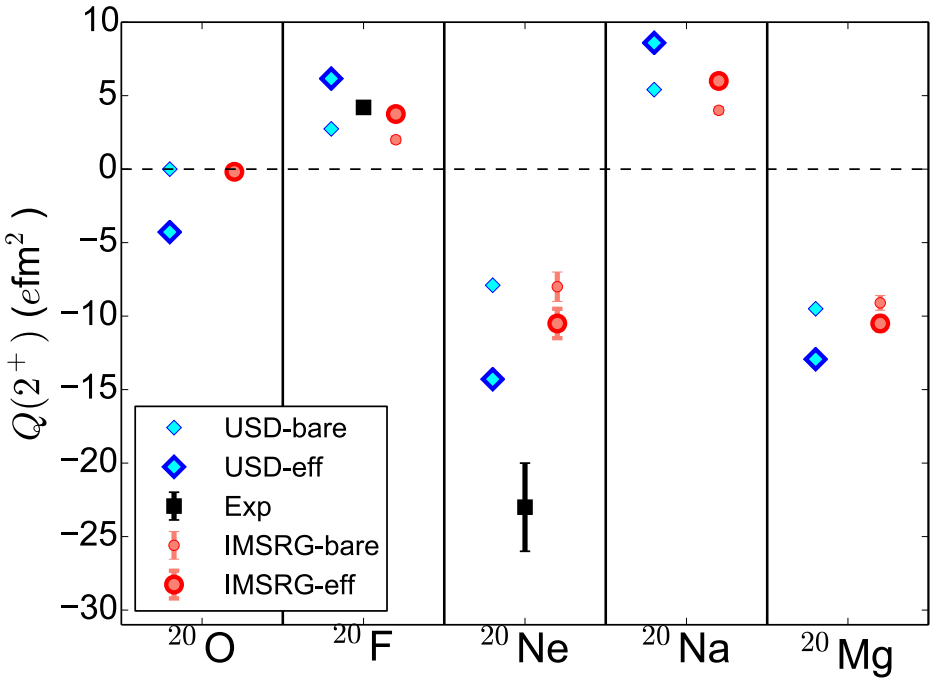
2-body part non-negligible

Ab Initio EM Moments

Calculate ab initio EM moments for all sd-shell nuclei

Compare with phenomenological USDB: quenching and effective charges





Stroberg et al., in prep

Modest effect from renormalized effective operator

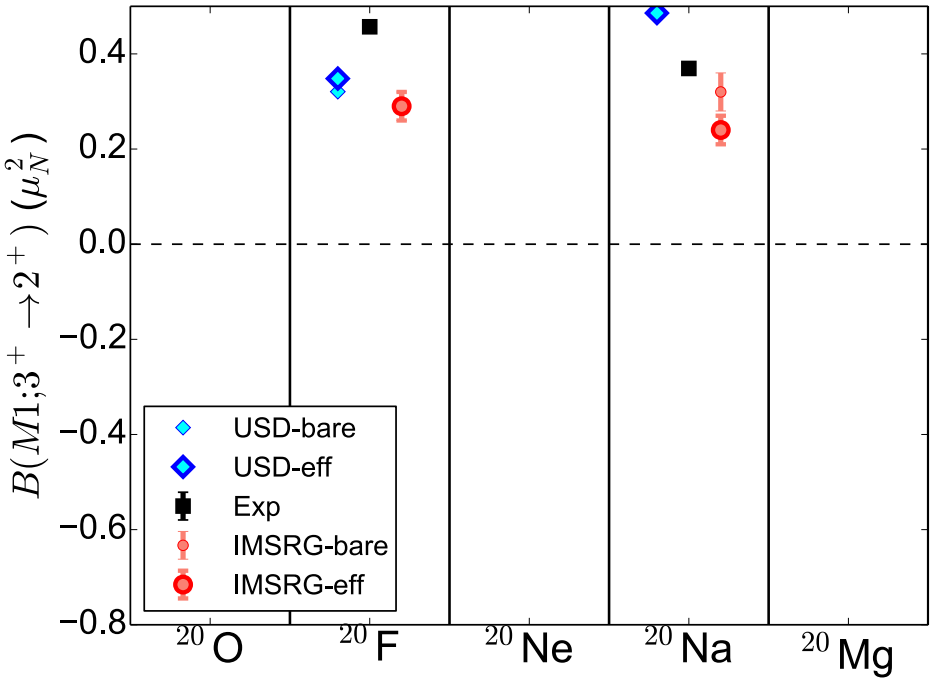
Magnetic moments agree with data and USDB (missing current corrections)

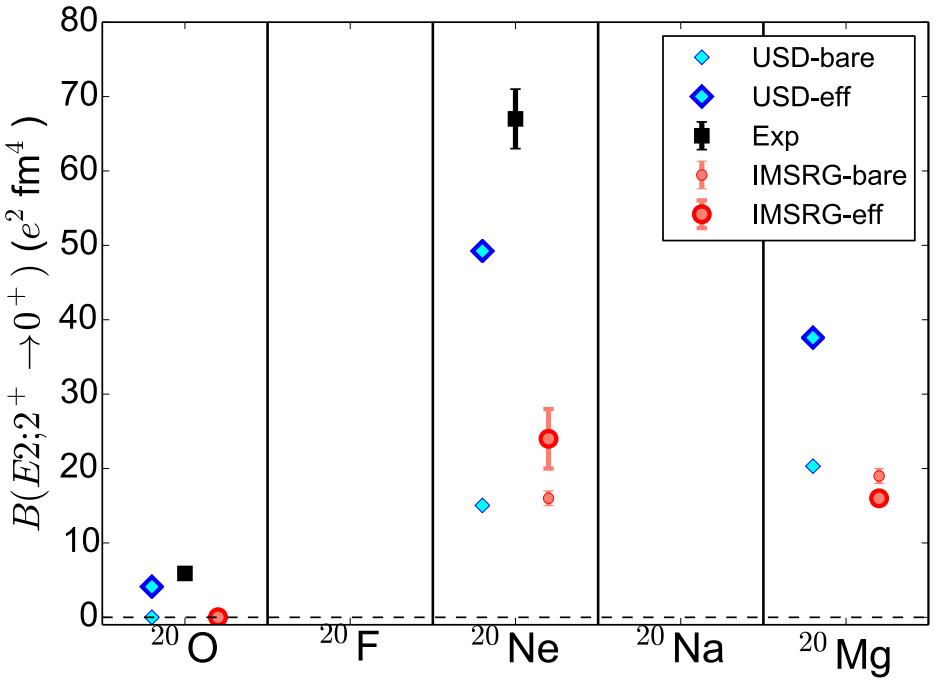
Electric quadrupole moments more problematic

Ab Initio EM Transition Rates

Calculate ab initio EM transition rates for full sd shell

Compare with phenomenological USDB: quenching and effective charges





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New Directions and Outlook

Heavier semi-magic chains: MBPT as guide

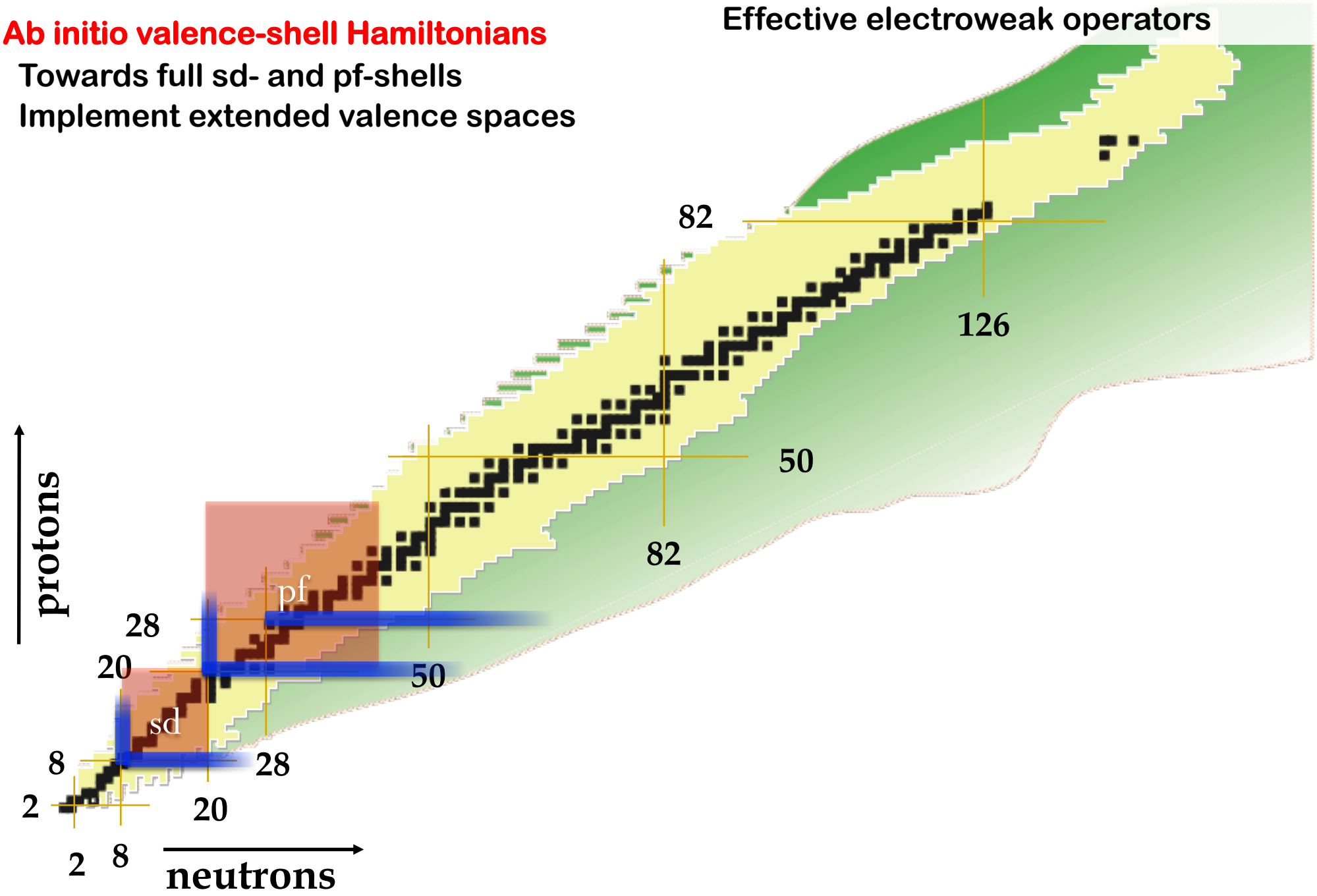
Ab initio valence-shell Hamiltonians

Towards full sd- and pf-shells

Implement extended valence spaces

Fundamental symmetries

Effective electroweak operators



New Directions and Outlook

Heavier semi-magic chains: MBPT as guide

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Implement extended valence spaces

Moving beyond stability

Include continuum effects

Map sd- and pf-shell driplines?

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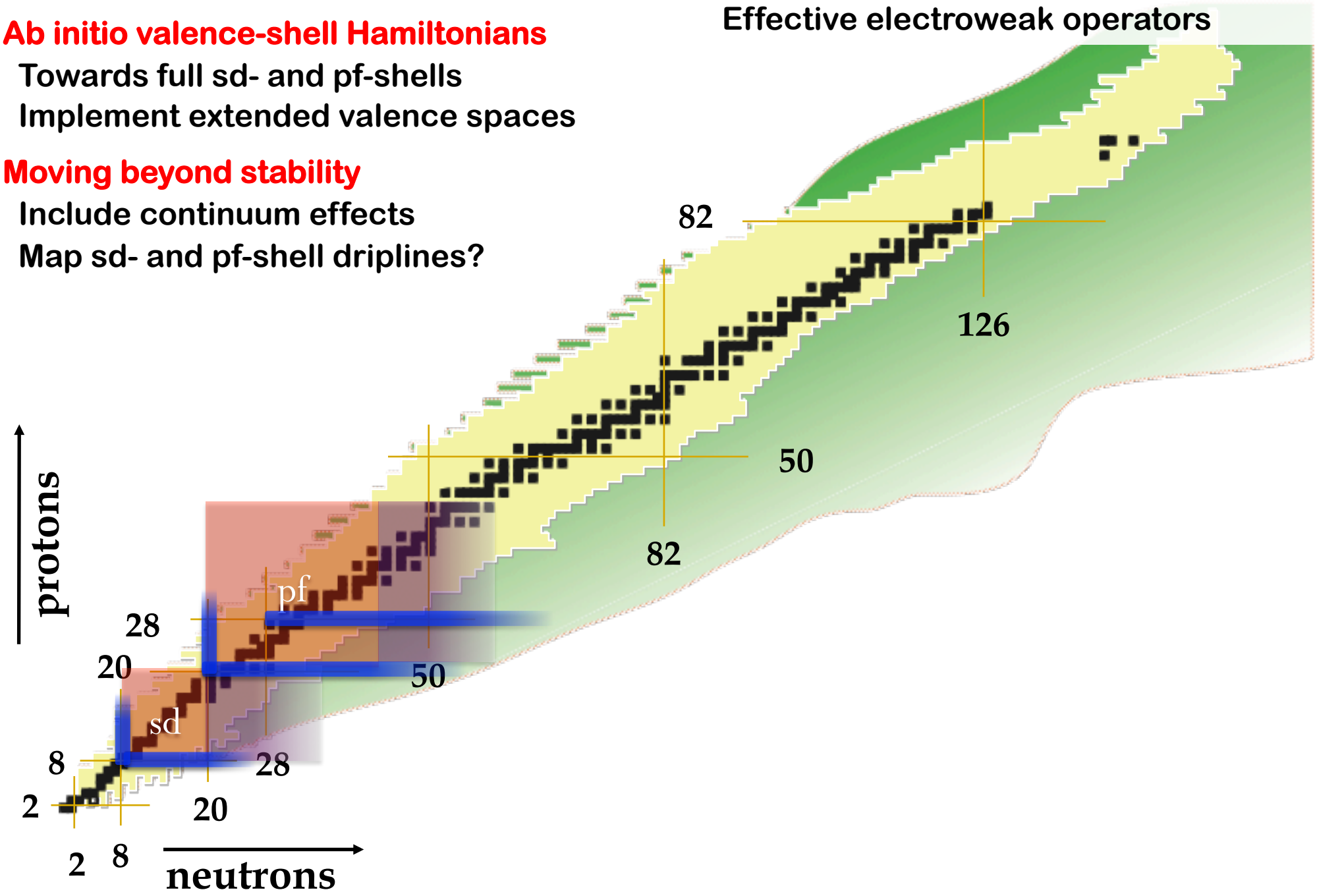

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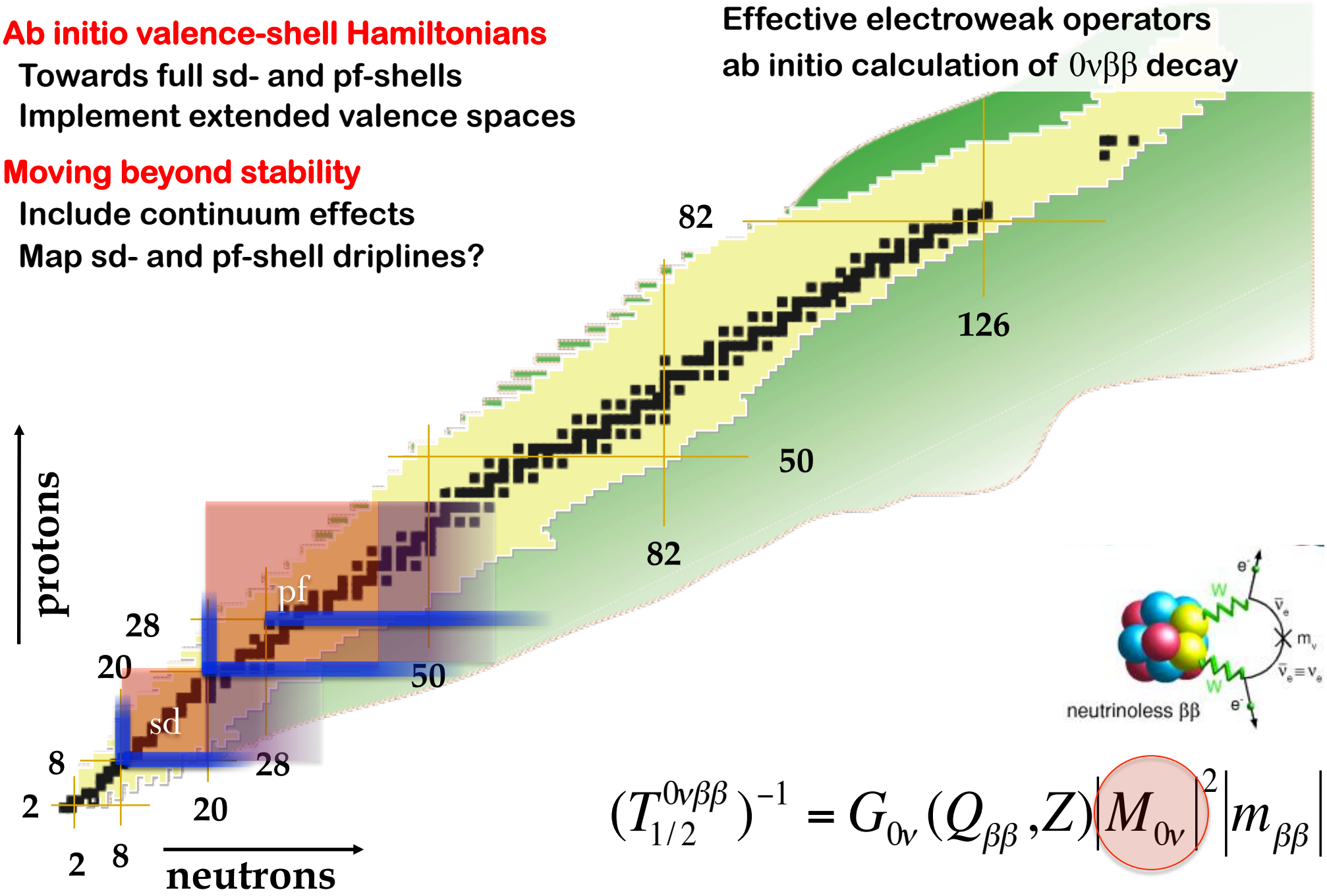
ab initio calculation of $0\nu\beta\beta$ decay



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