New Directions in Valence-Space Methods for Exotic sd-Shell Nuclei

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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, Binder, Calci, Langhammer, Roth, arXiv:1402.1407

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

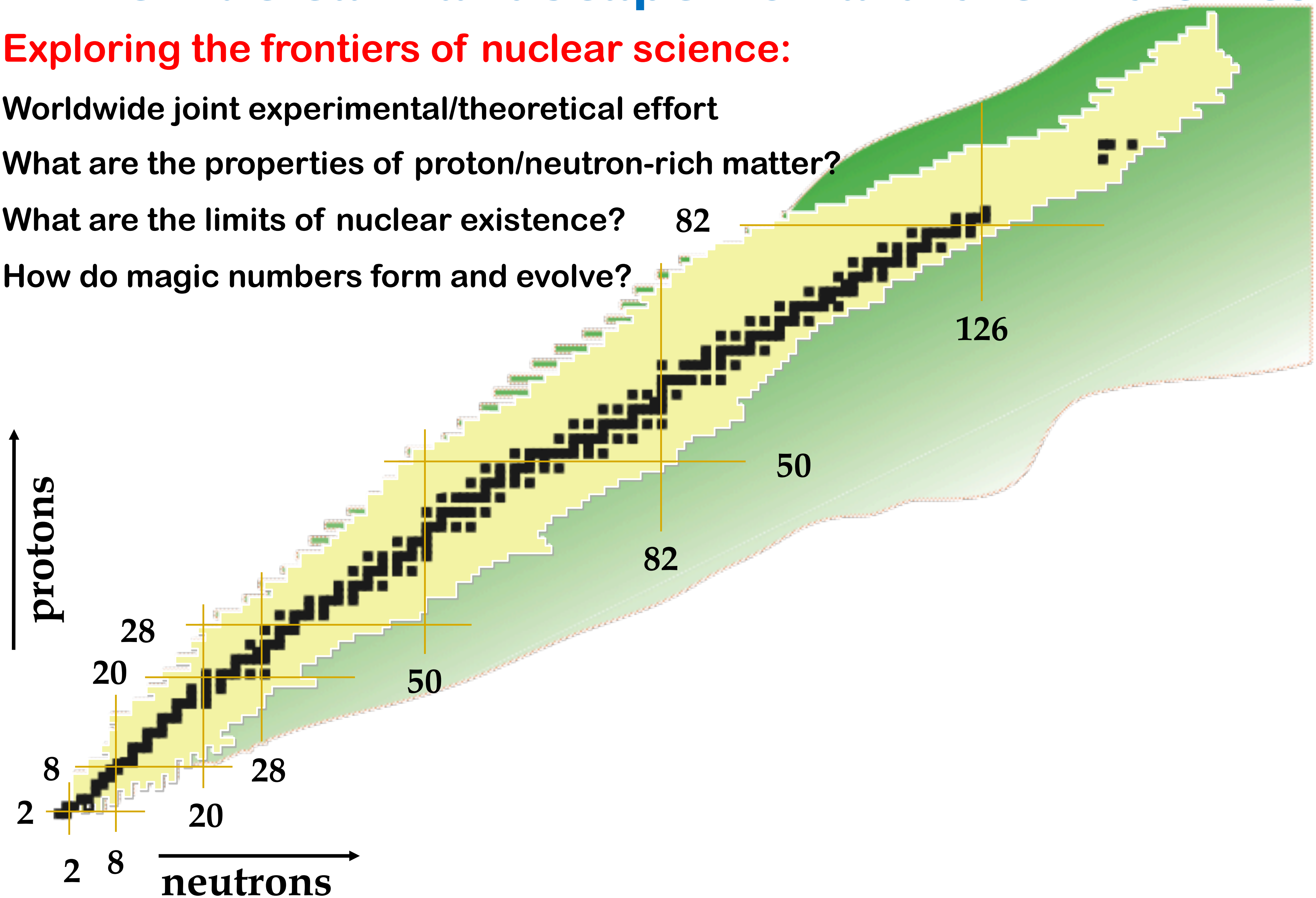
Exploring the frontiers of nuclear science:

Worldwide joint experimental/theoretical effort

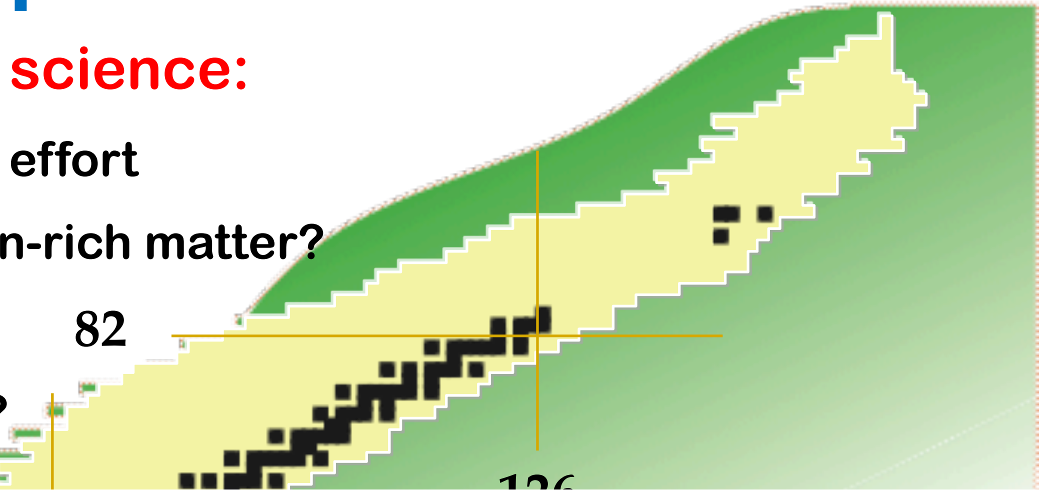
What are the properties of proton/neutron-rich matter?

What are the limits of nuclear existence?

How do magic numbers form and evolve?



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



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Advances in many-body methods

Green's Function Monte Carlo

Hyperspherical Harmonics

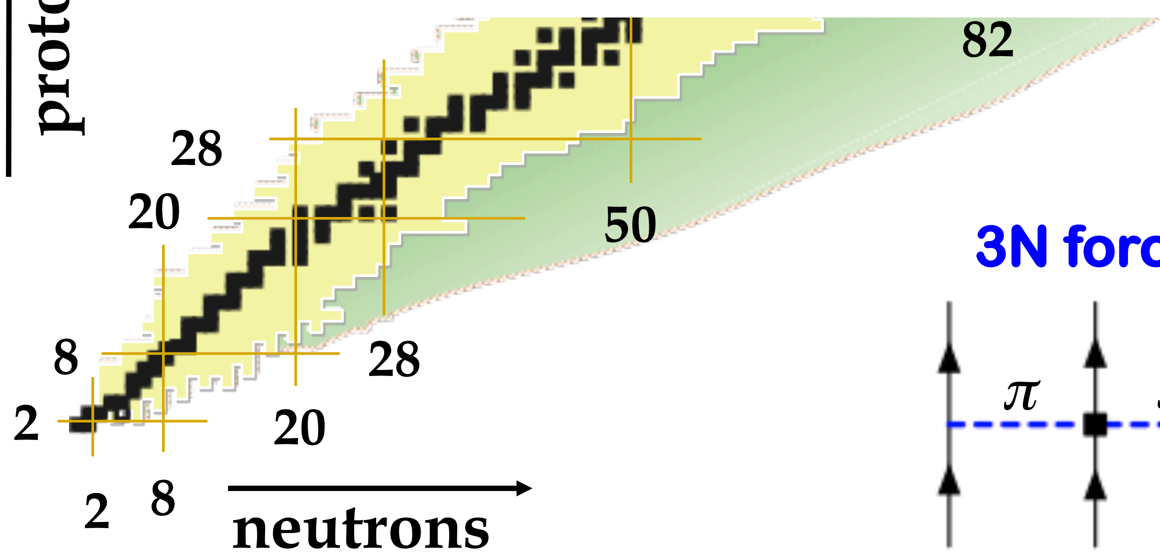
(IT) No-Core Shell Model

Coupled Cluster

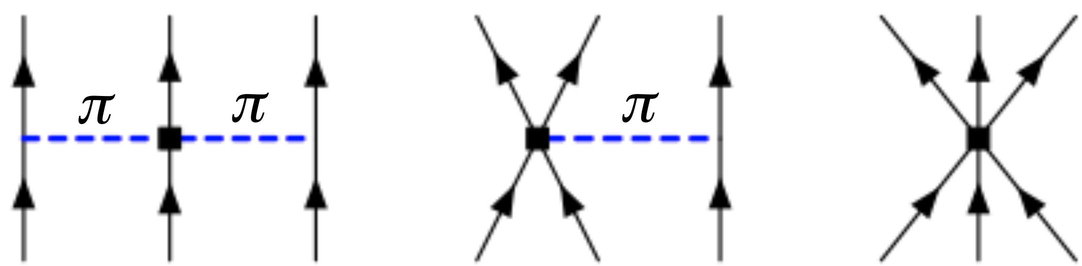
In-Medium SRG

Many-Body Perturbation Theory

Self-Consistent Green's Function



3N forces essential for exotic nuclei



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

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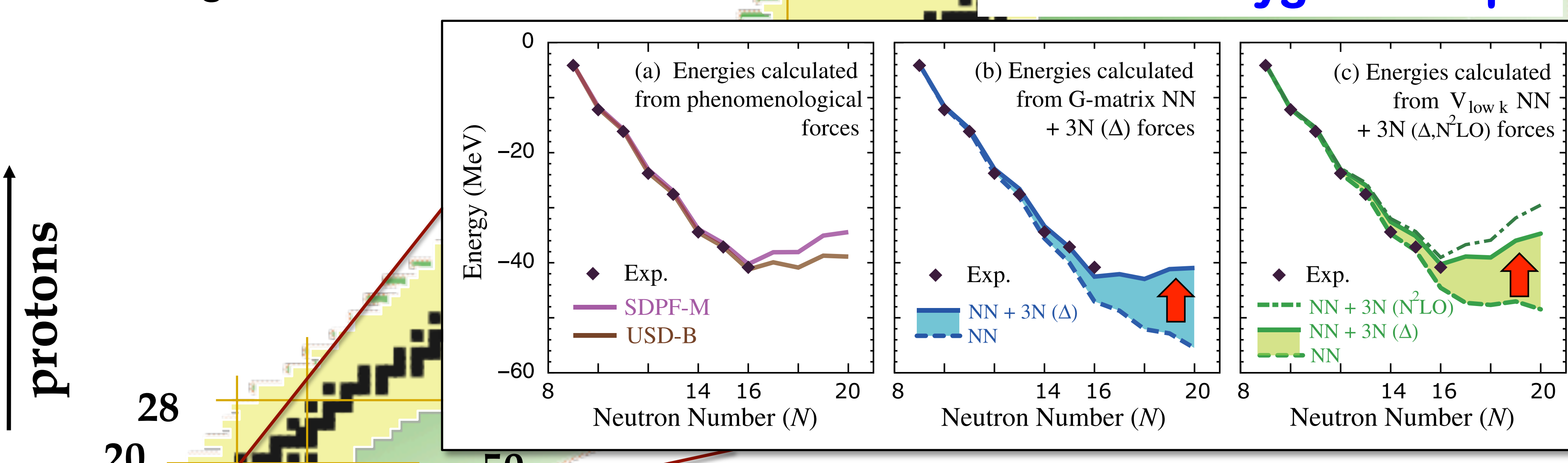
Heaviest oxygen isotope



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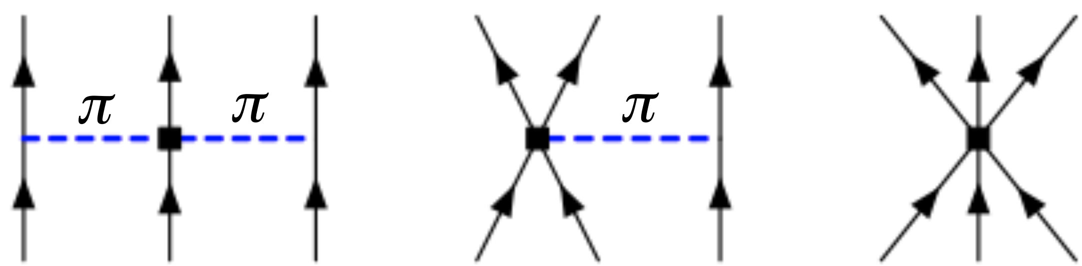

Drip Lines and Magic Numbers: 3N Forces in Medium-Mass Nuclei

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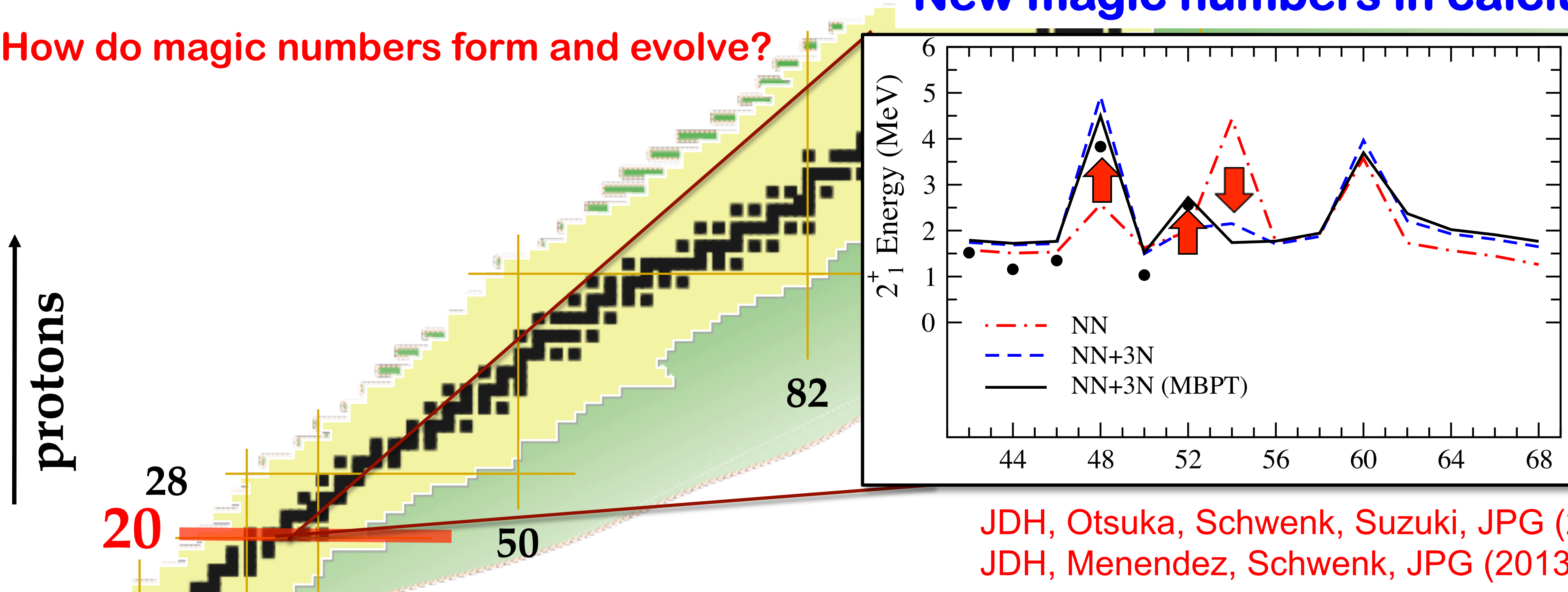
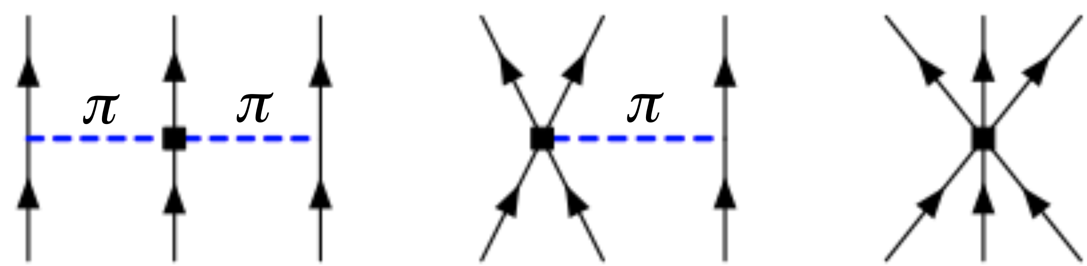
New magic numbers in calcium



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



Oxygen Isotopes

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Worldwide joint experimental/theoretical effort

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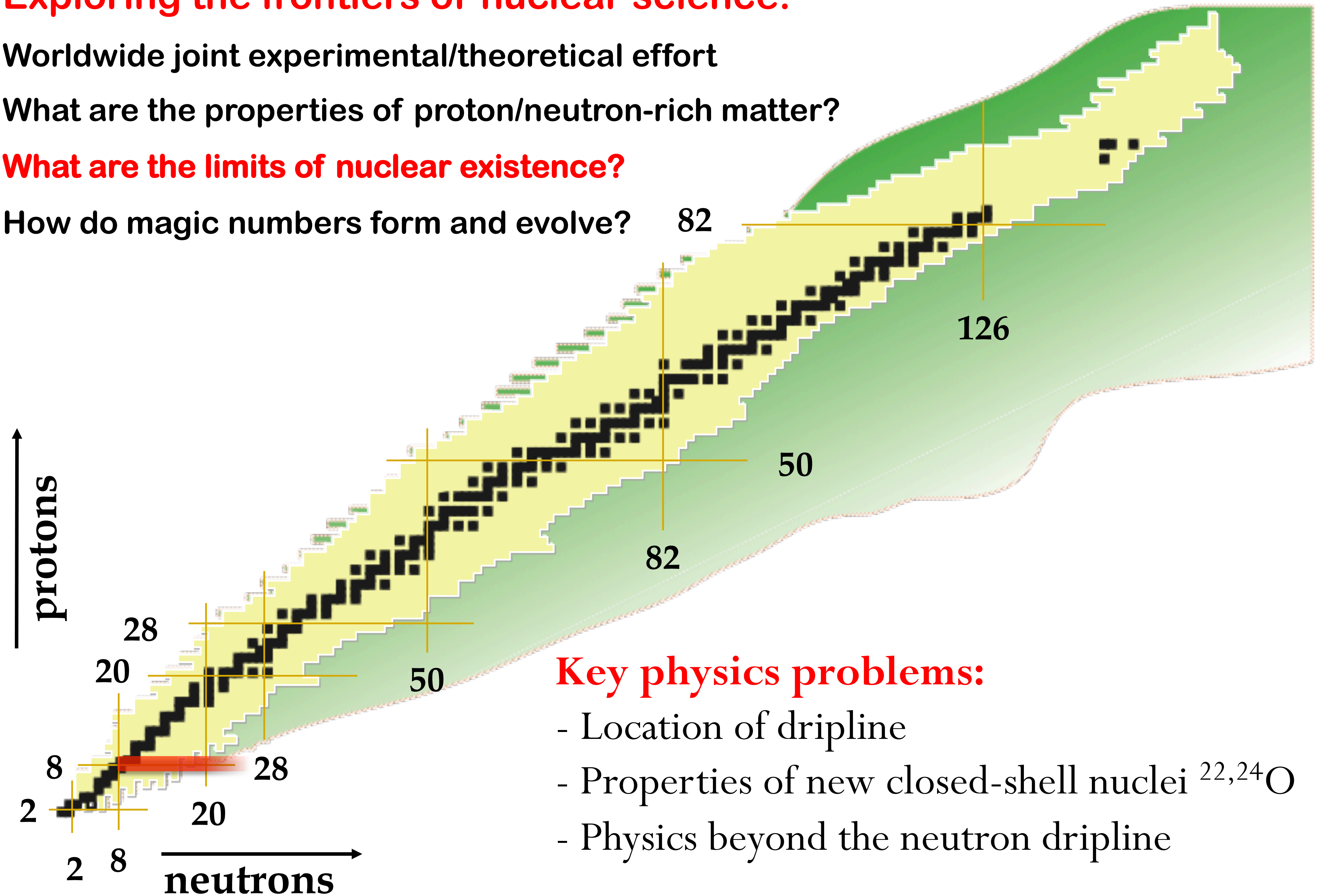


Key physics problems:

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

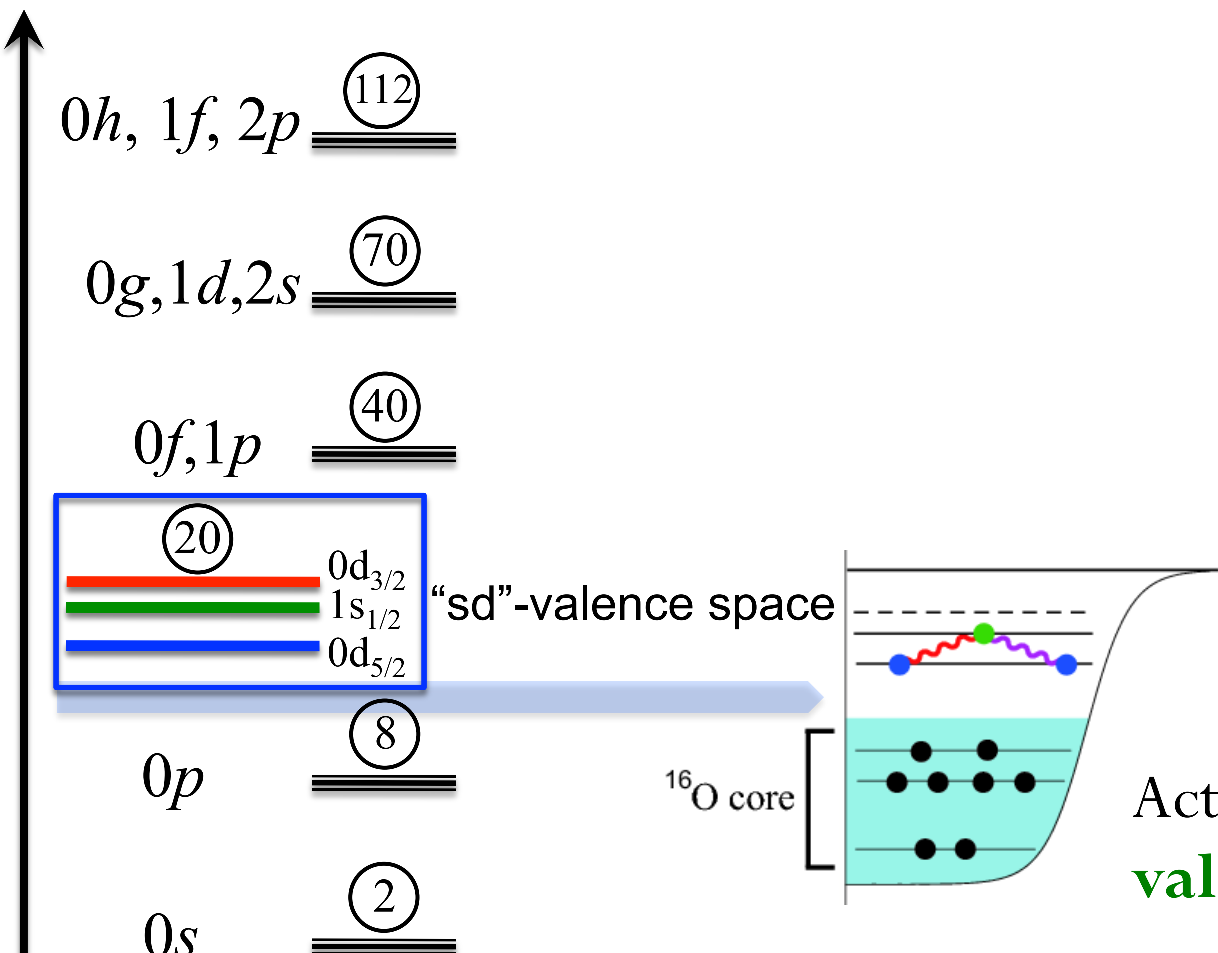
The Nuclear Many-Body Problem

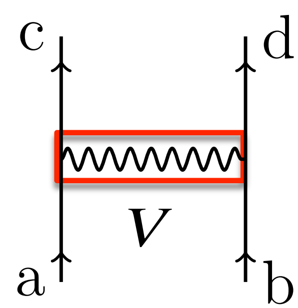
Nuclei understood as many-body system starting from closed shell, add nucleons

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

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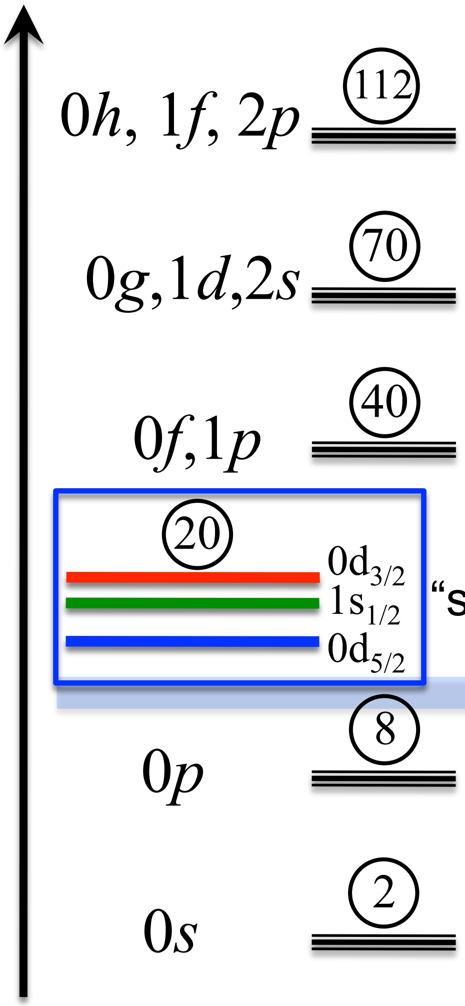
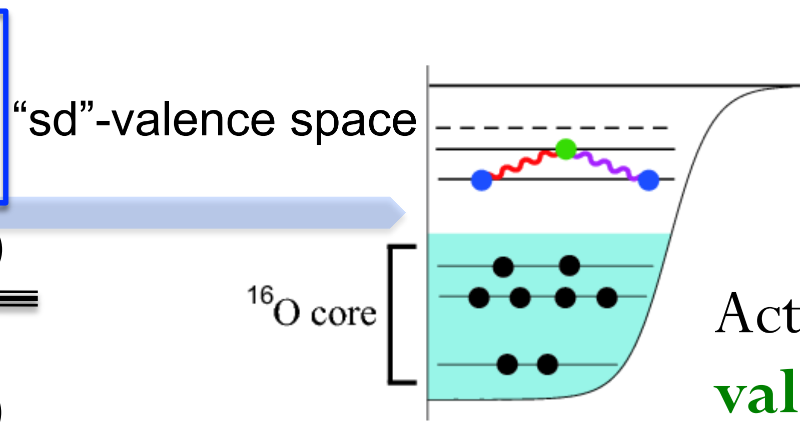
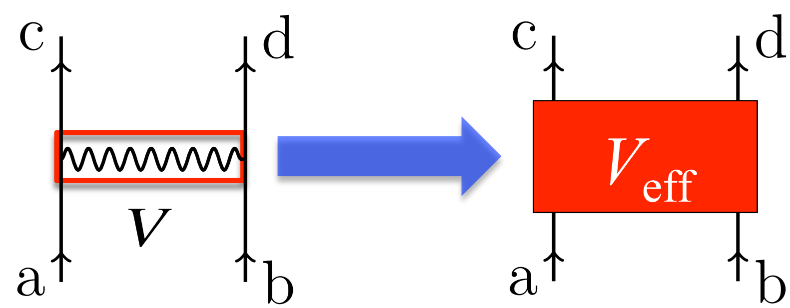


Solution: allow breaking of core

Effective Hamiltonian for valence nucleons





Active nucleons occupy **valence space**

Valence-Space Strategy

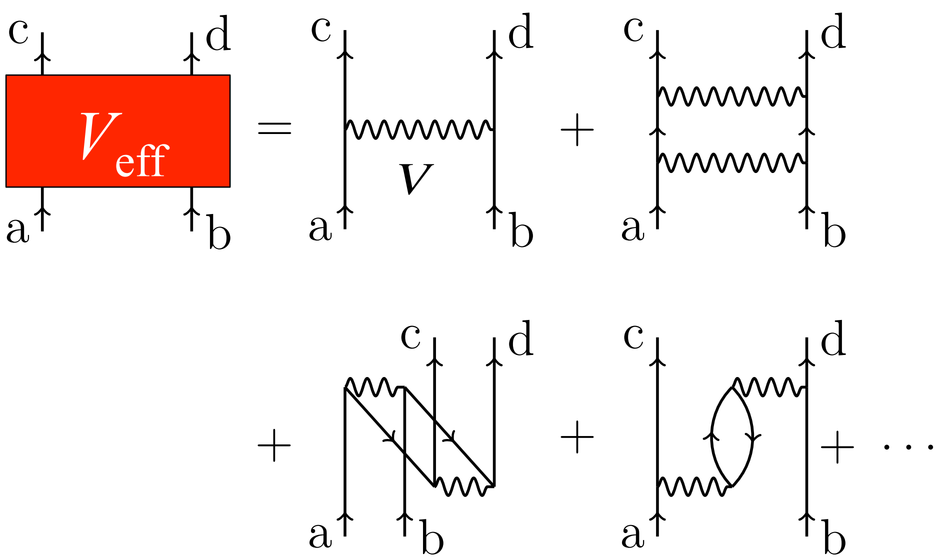
★ 1) Effective interaction: sum excitations outside valence space to **3rd order**

★ 2) Single-particle energies calculated self consistently

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

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

5) Explore extended valence spaces



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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

Valence-Space Strategy

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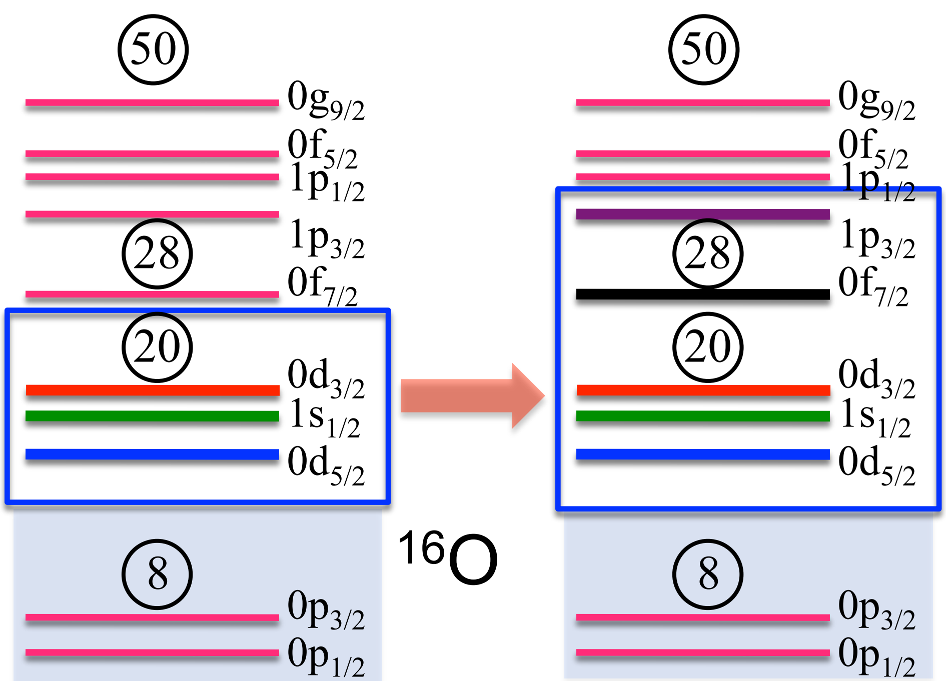
★ 5) Explore **extended valence spaces**

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



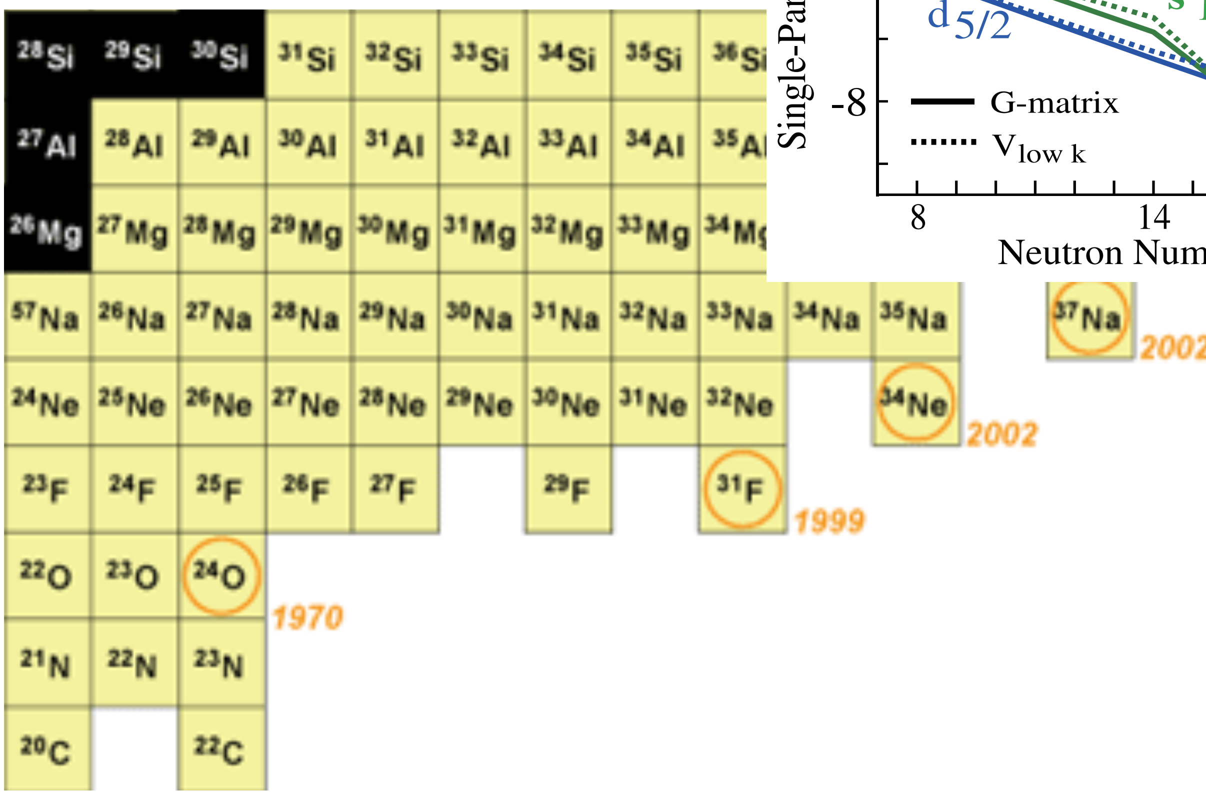
Treats higher orbits nonperturbatively

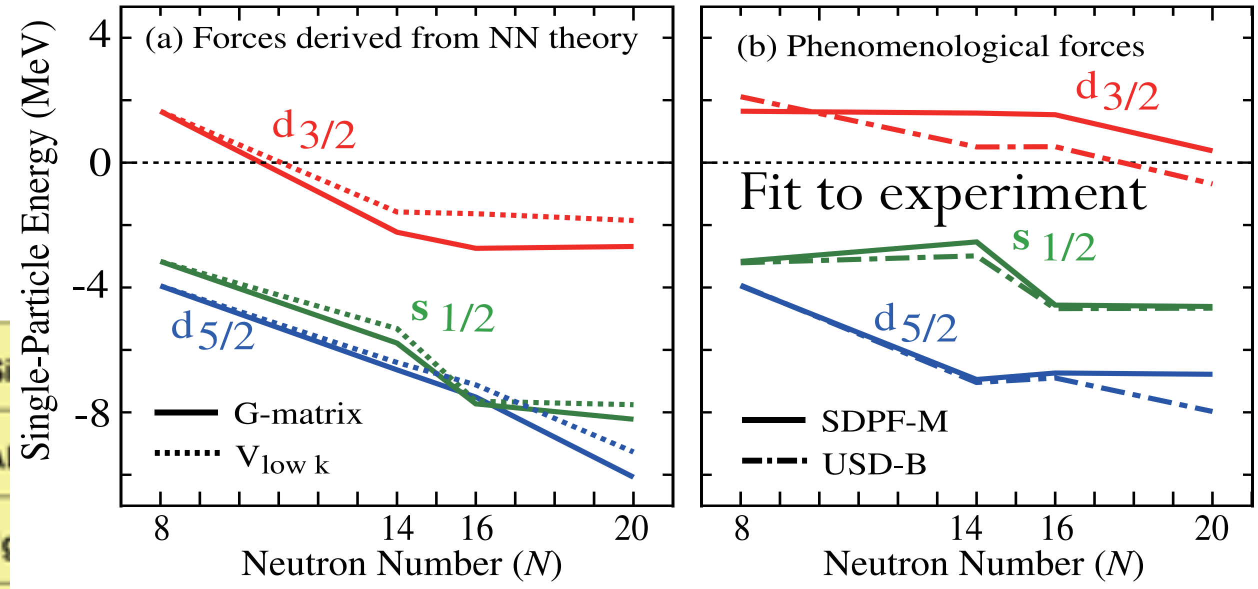
When important for exotic nuclei?

Limits of Nuclear Existence: Oxygen Anomaly

Microscopic picture:

NN-forces too attractive





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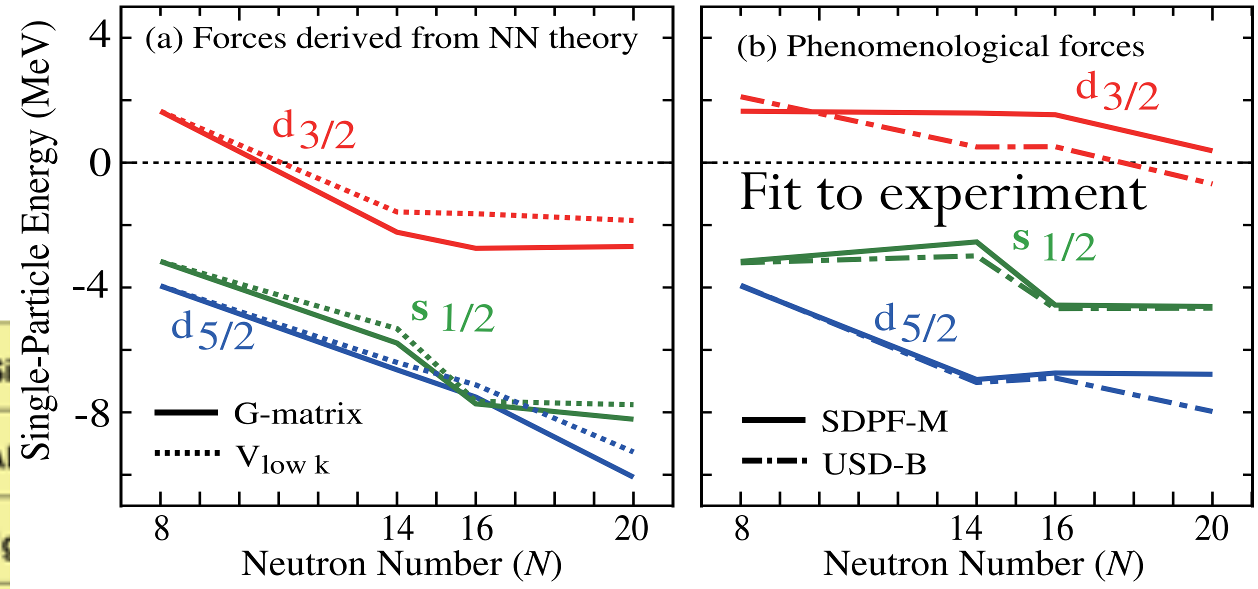

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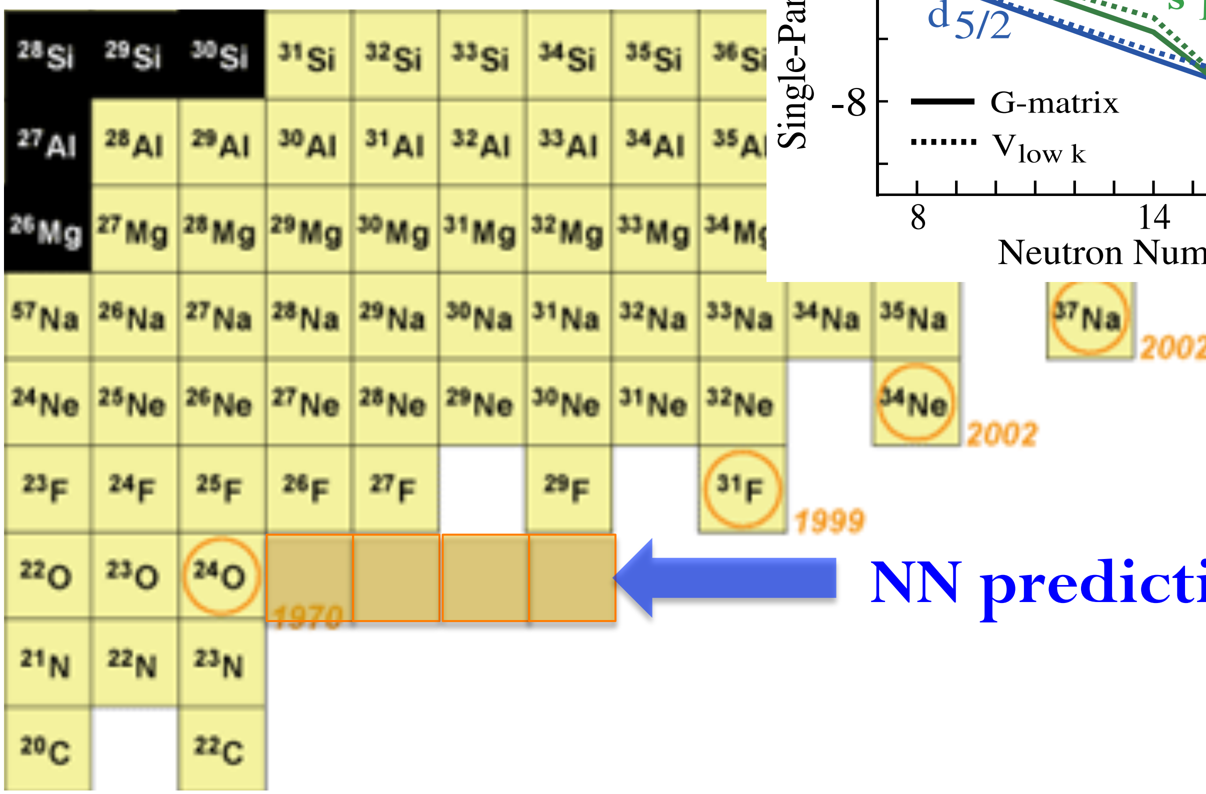
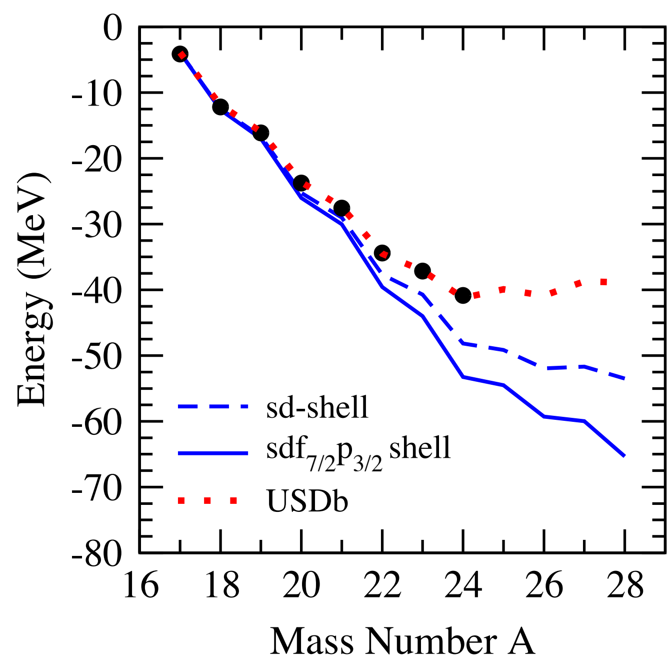
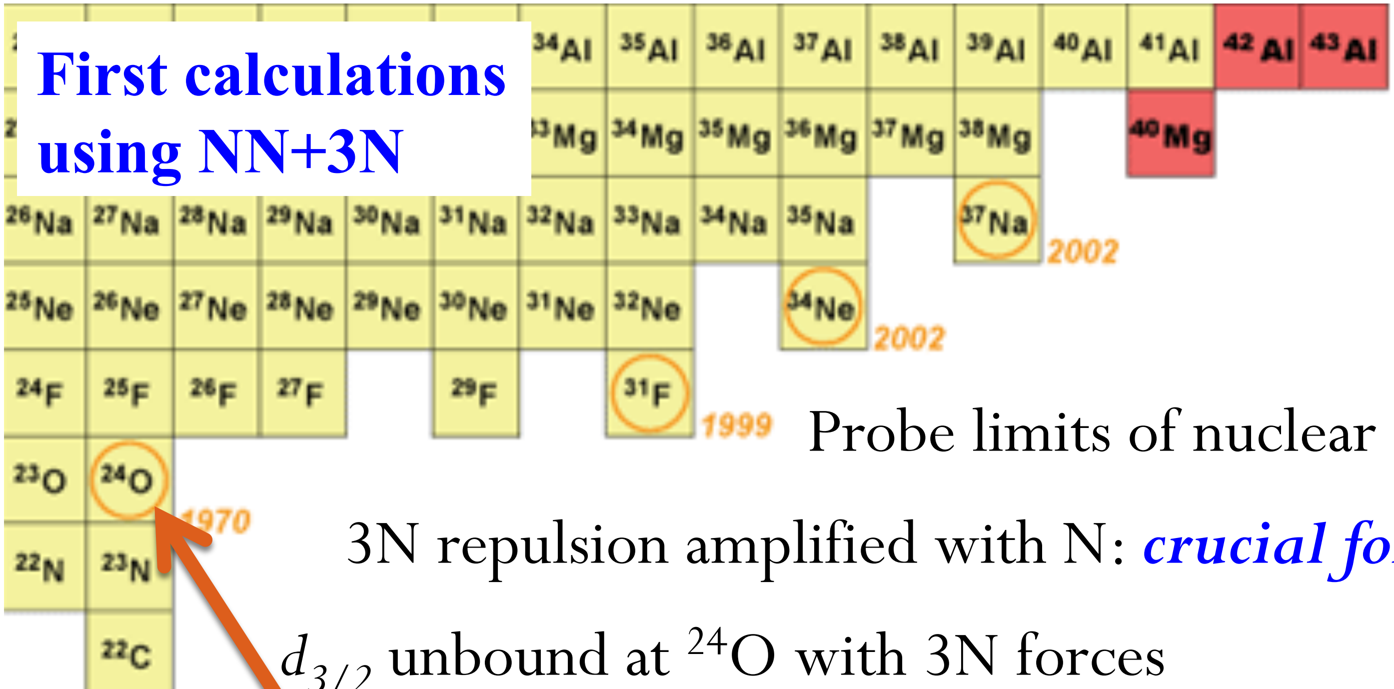




Incorrect prediction of oxygen dripline

Extended-space – more binding

Oxygen Anomaly

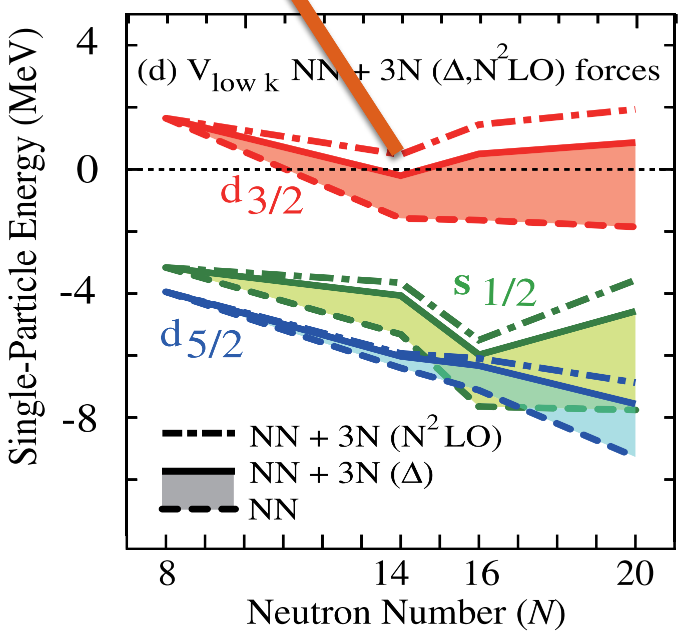


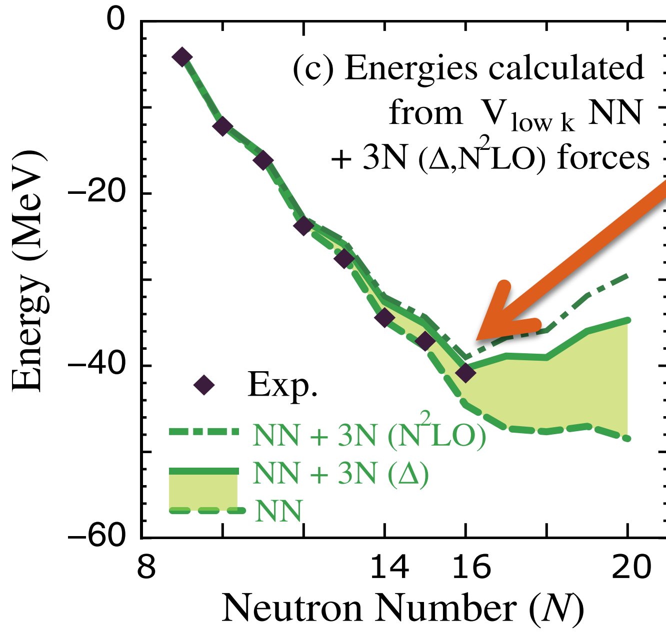
First calculations using NN+3N

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





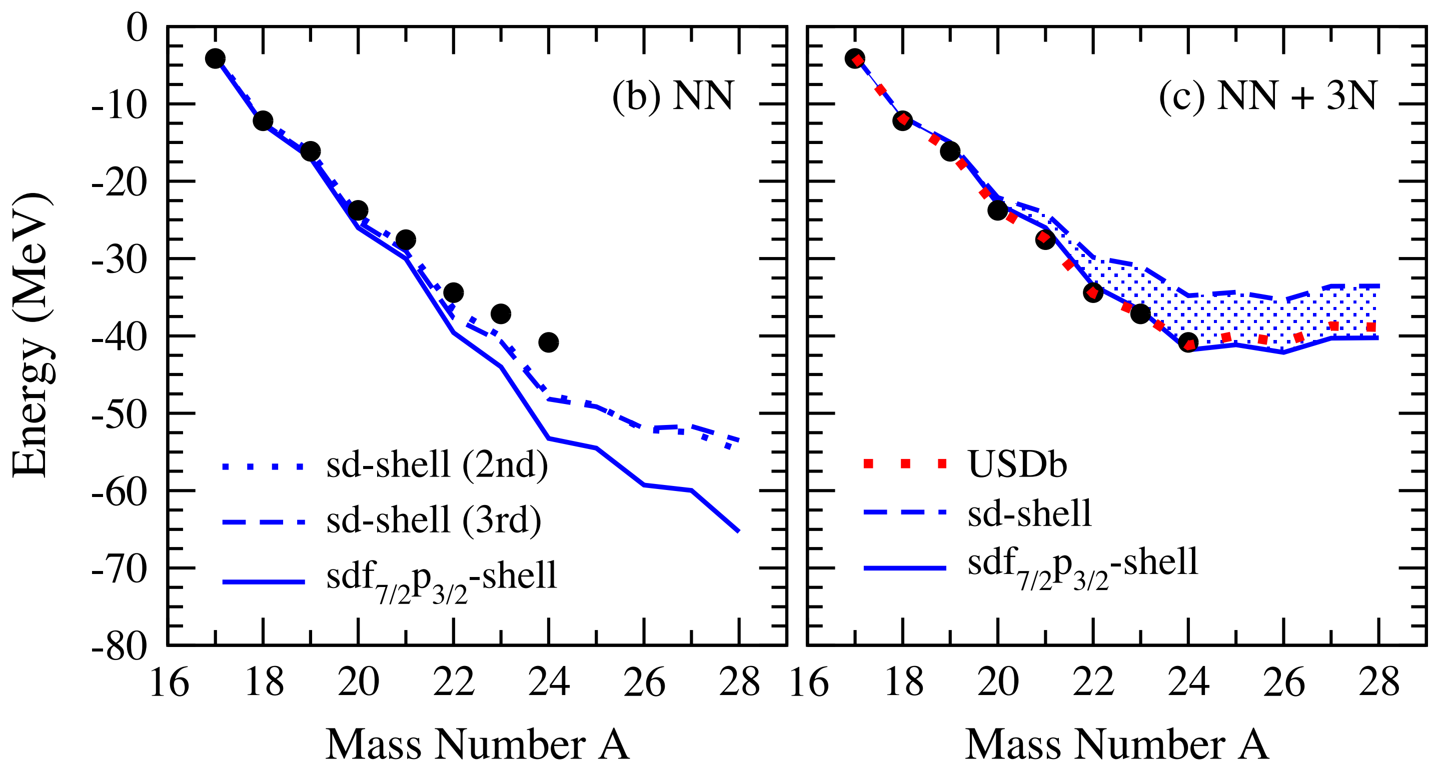
Isotopes unbound beyond ^{24}O

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)

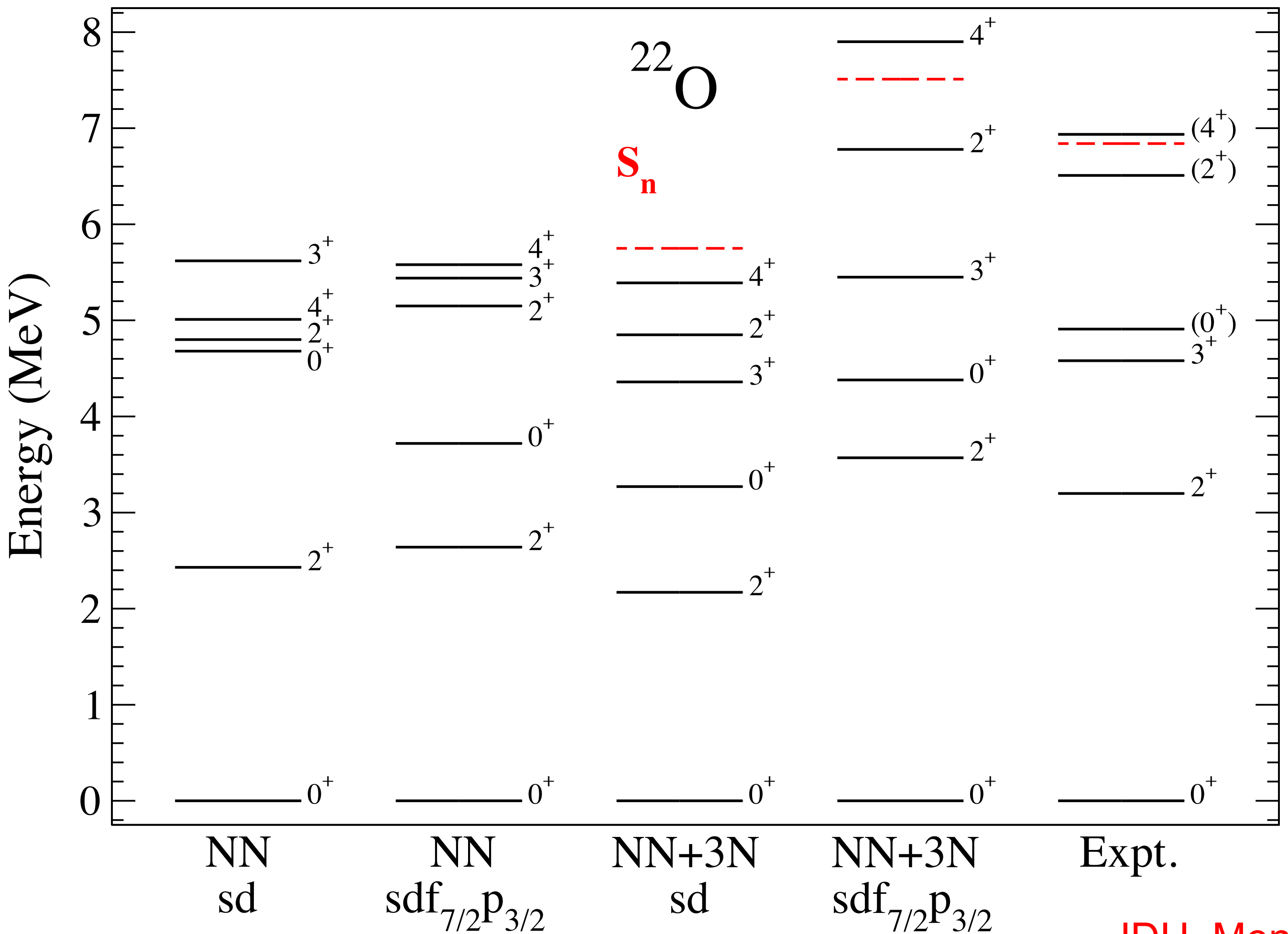
Repulsive character improves agreement with experiment

sd-shell results underbound; improved in **extended space**

Impact on Spectra: ^{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

NN+3N

Extended space essential

Reproduces $N=14$ magic number

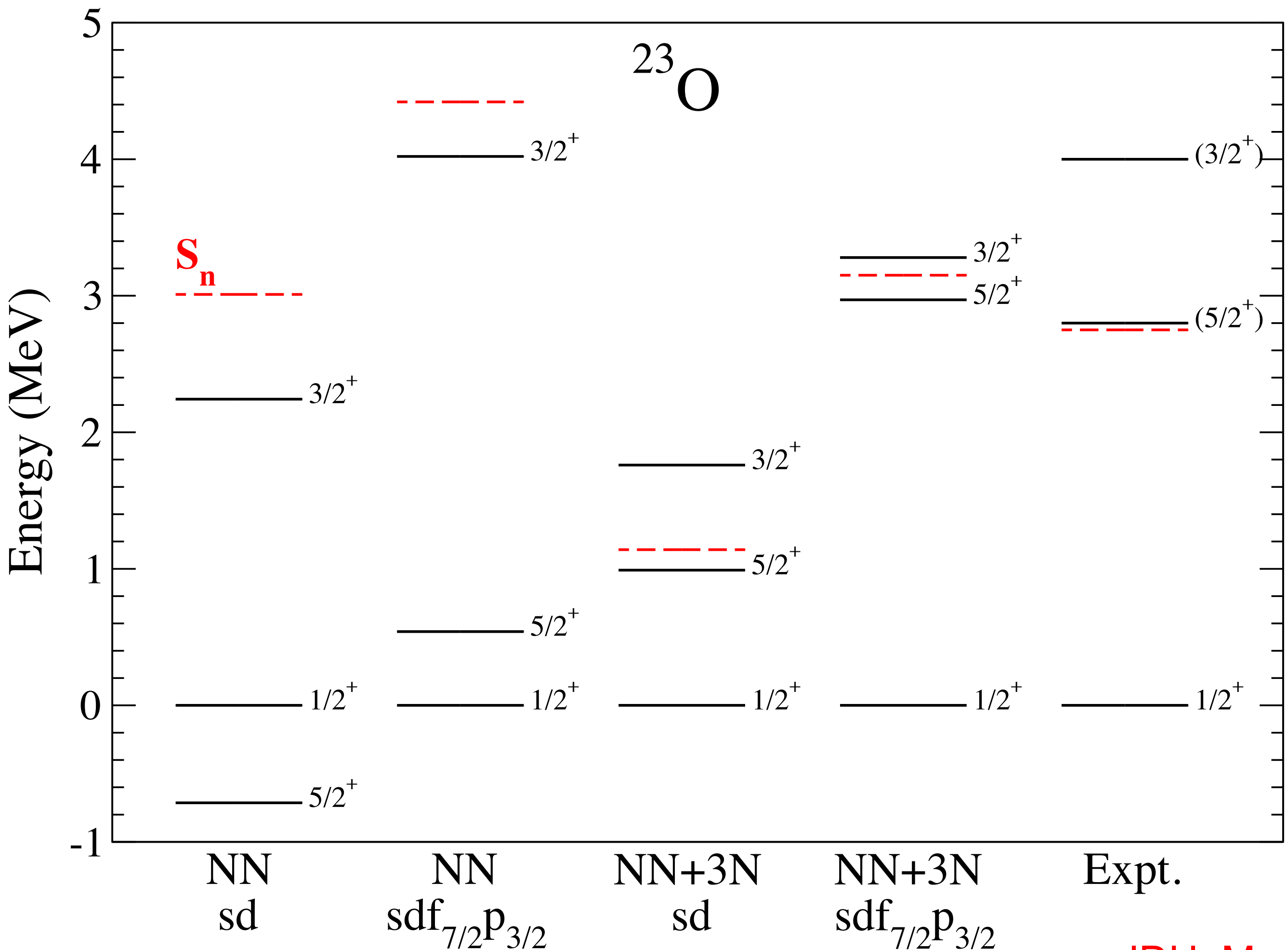
JDH, Menendez, Schwenk, EPJA (2013)

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

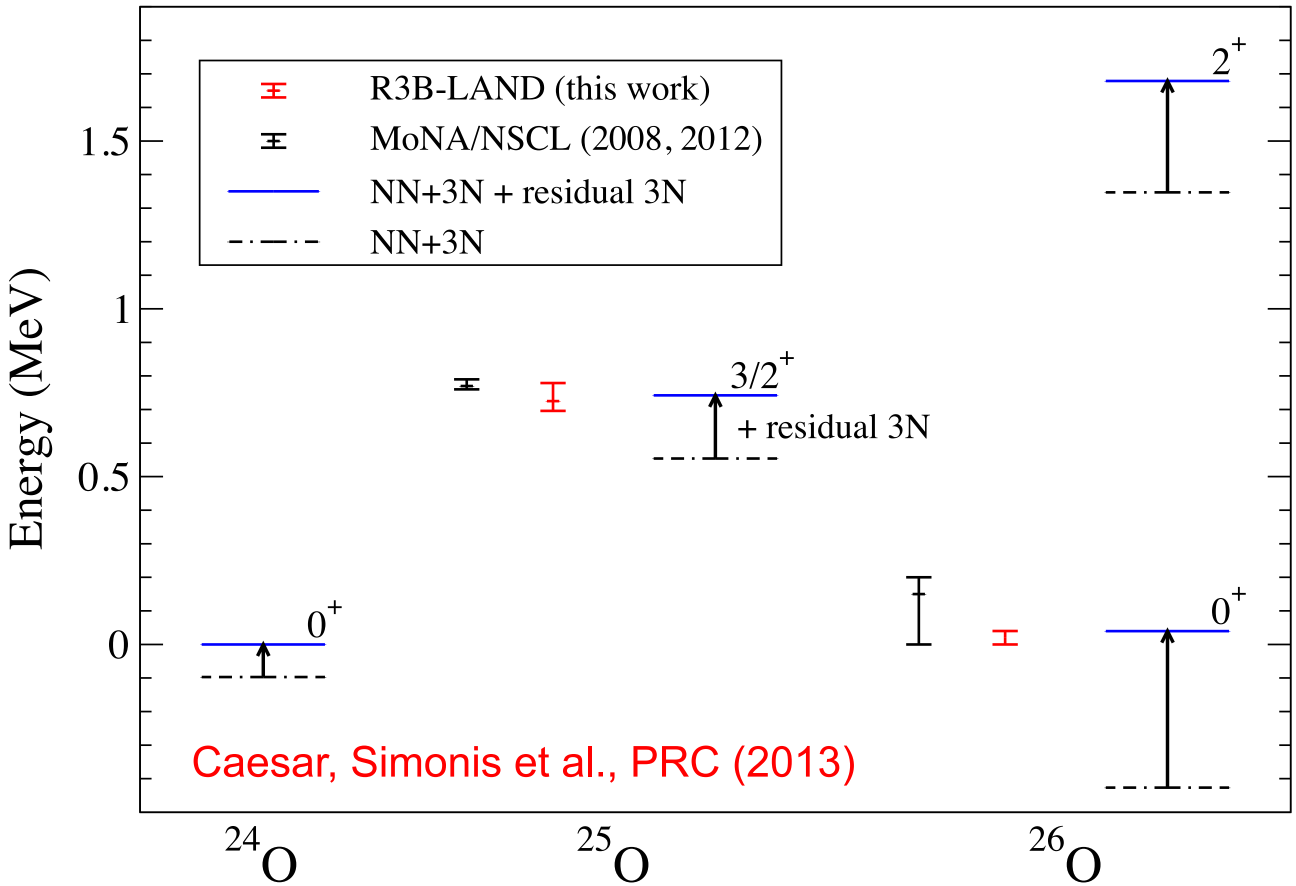
Clear improvement in extended valence space

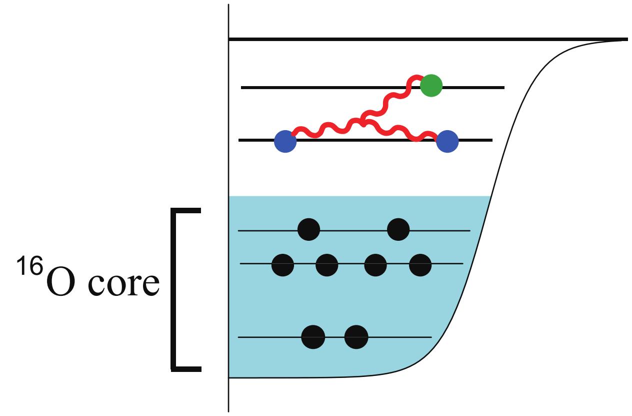
JDH, Menendez, Schwenk, EPJA (2013)

Experimental Connection: Beyond the Dripline

Hoffman, Kanungo, Lunderberg… PRLs (2008+)

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





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

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

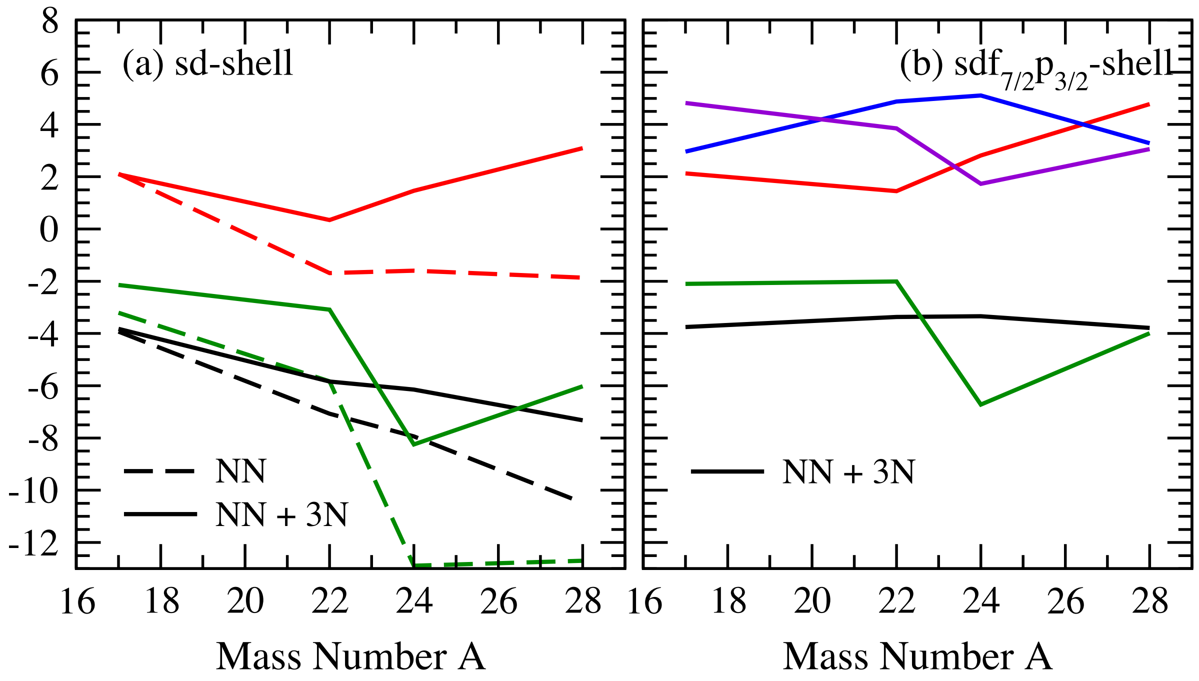
Repulsion more pronounced for neutron-rich systems: 400 keV at ^{26}O

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

Future: include coupling to continuum

Evolution of SPEs

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



NN+3N extended space:

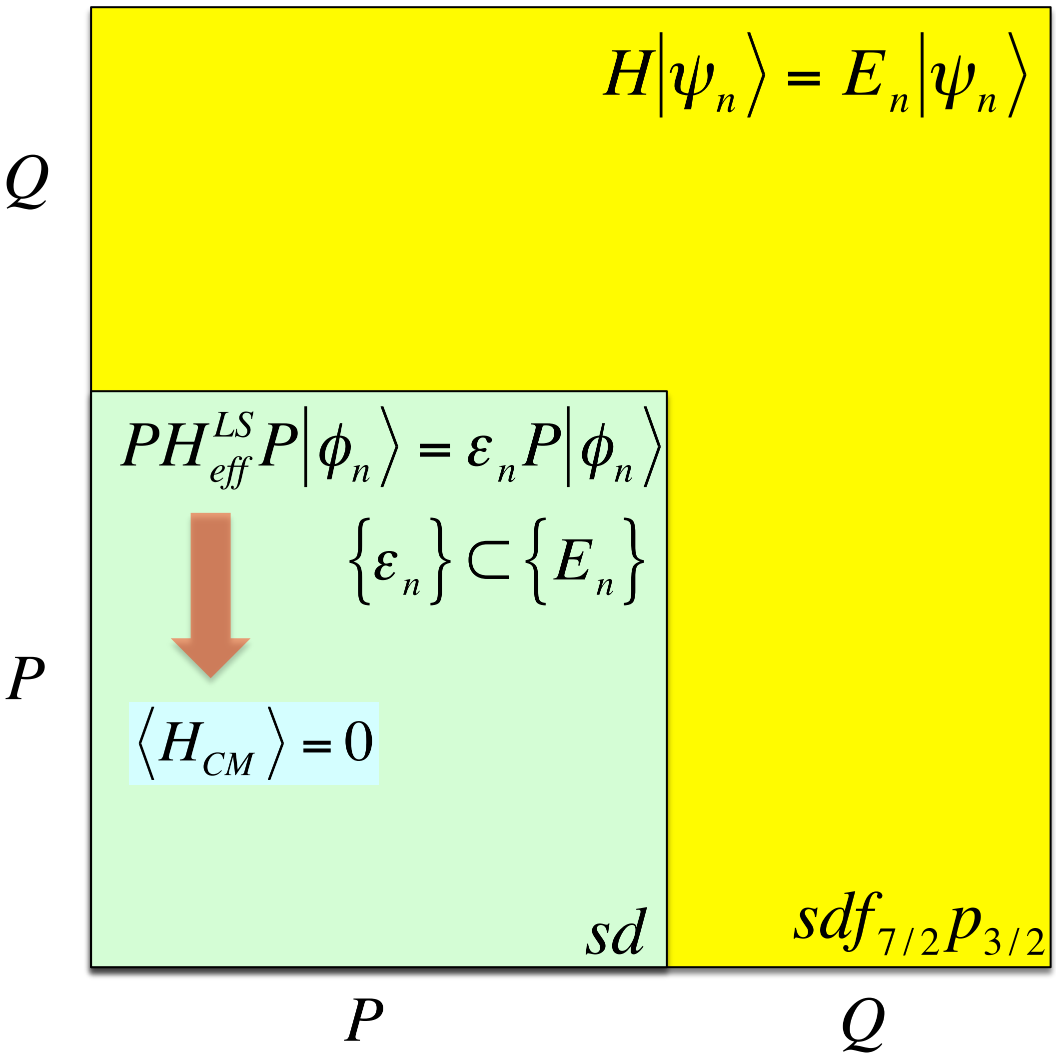
Much different trend than sd-shell

No gap at ^{22}O yet enhanced closed-shell features

Inversion of levels past ^{24}O – essential to include for neutron-rich oxygen

Evaluating Center-of-Mass Contamination

Nonperturbative Lee-Suzuki (LS) transformation from extended space

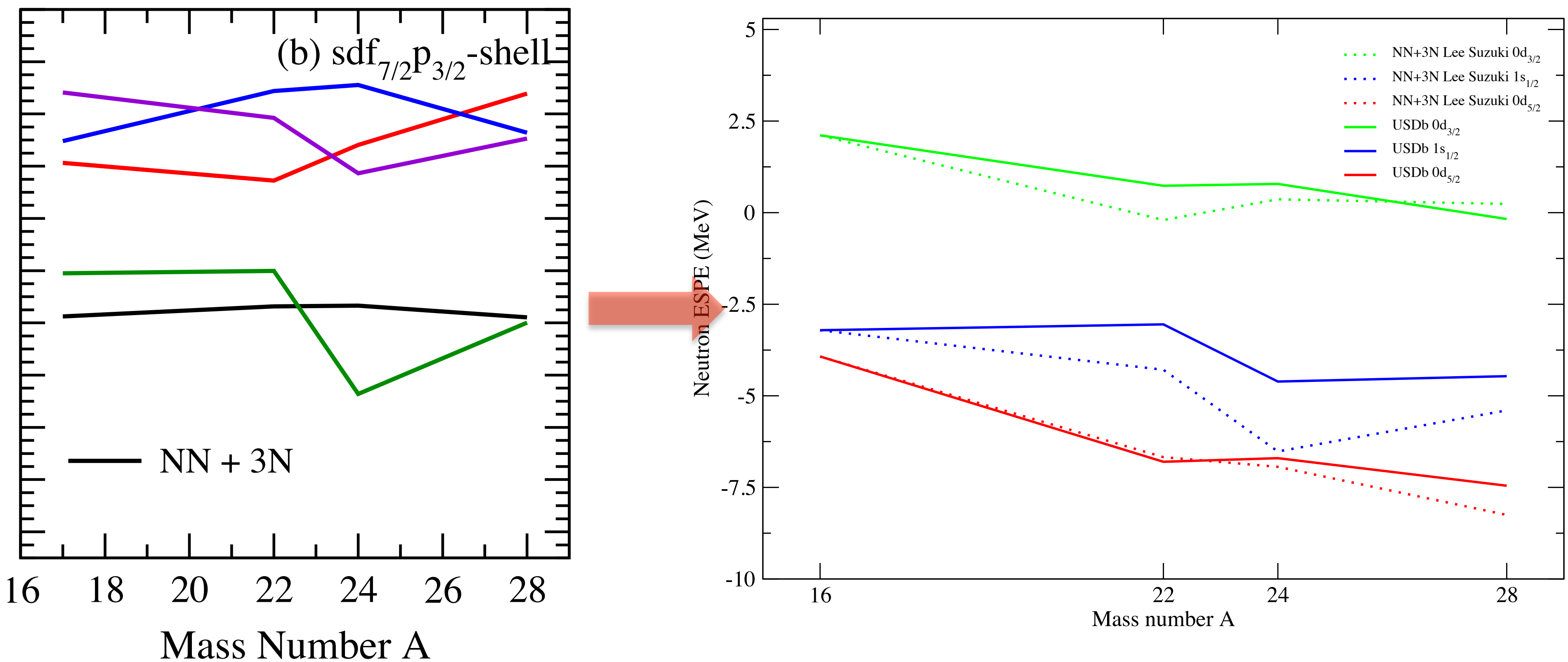


- Transform for **two-body** systems ($e.g.$, ^{18}O, ^{42}Ca)
- **Extended-space spectrum free of CM contamination**
- Project into standard space onto eigenenergies from extended space calculation

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

Evolution of SPEs

SPE evolution of LS-projected sd-shell interaction

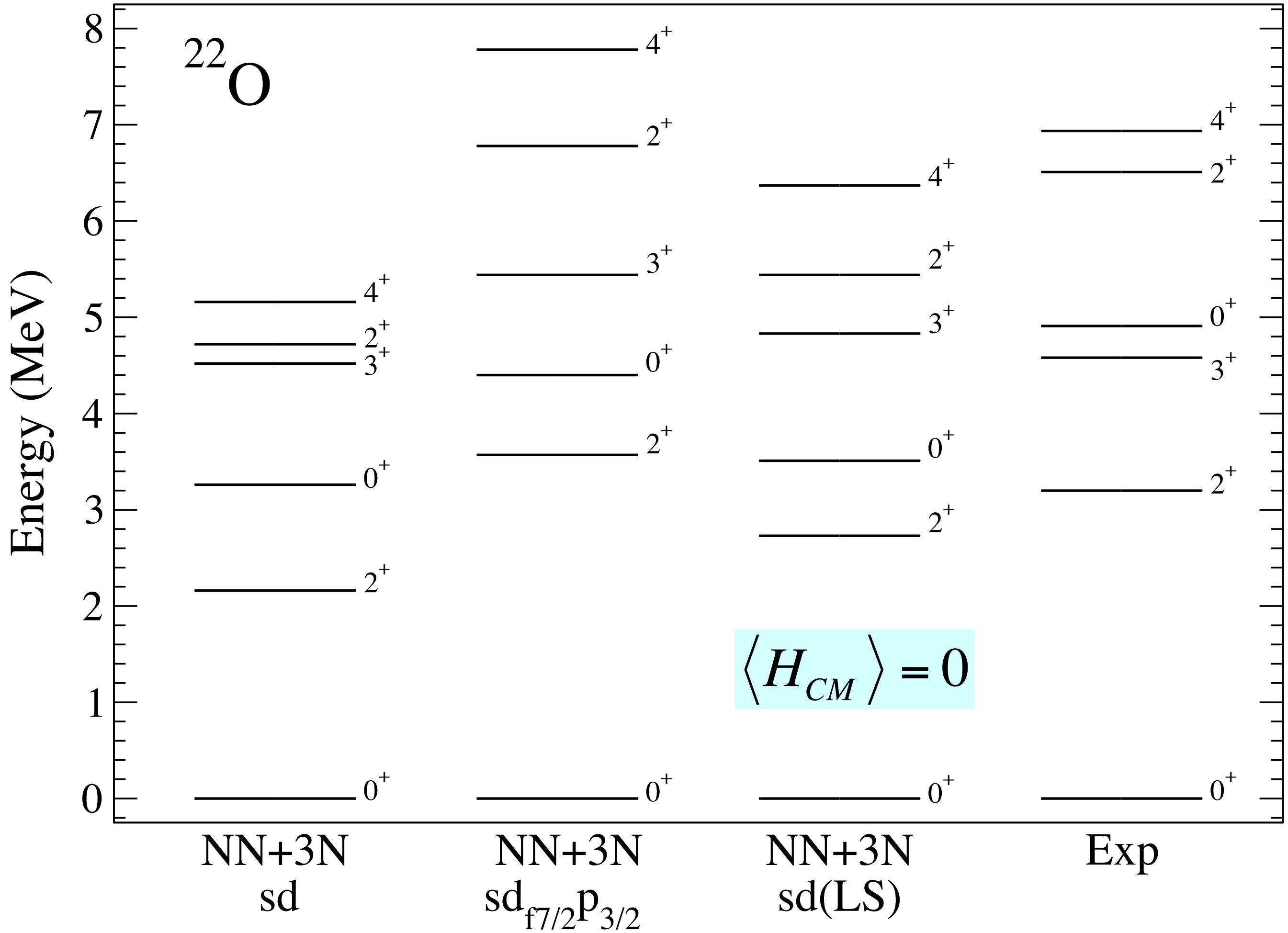


Overall evolution similar to USD – $s_{1/2}$ too attractive

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

Evaluating Center-of-Mass Contamination

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



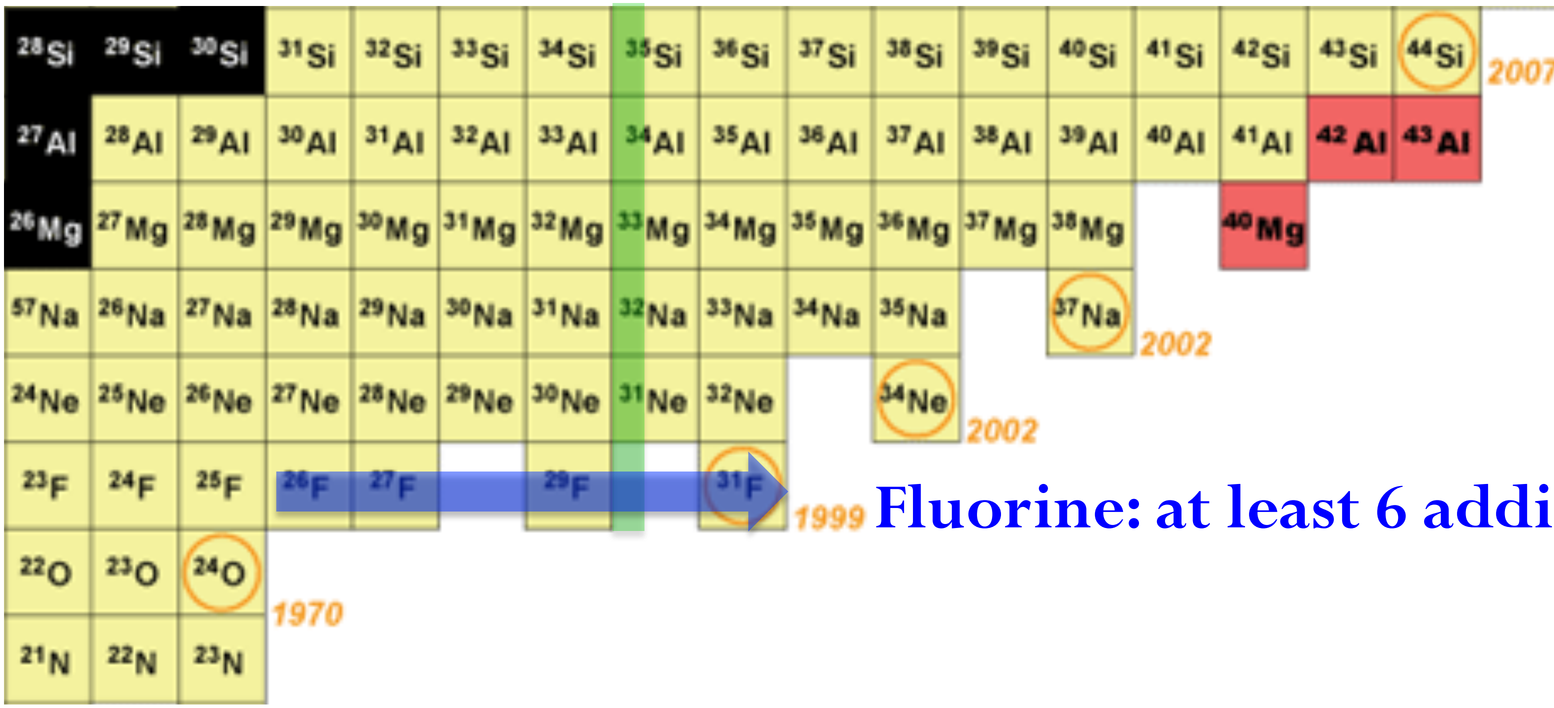
Improvements from standard *sd*-shell – not due to center of mass

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

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

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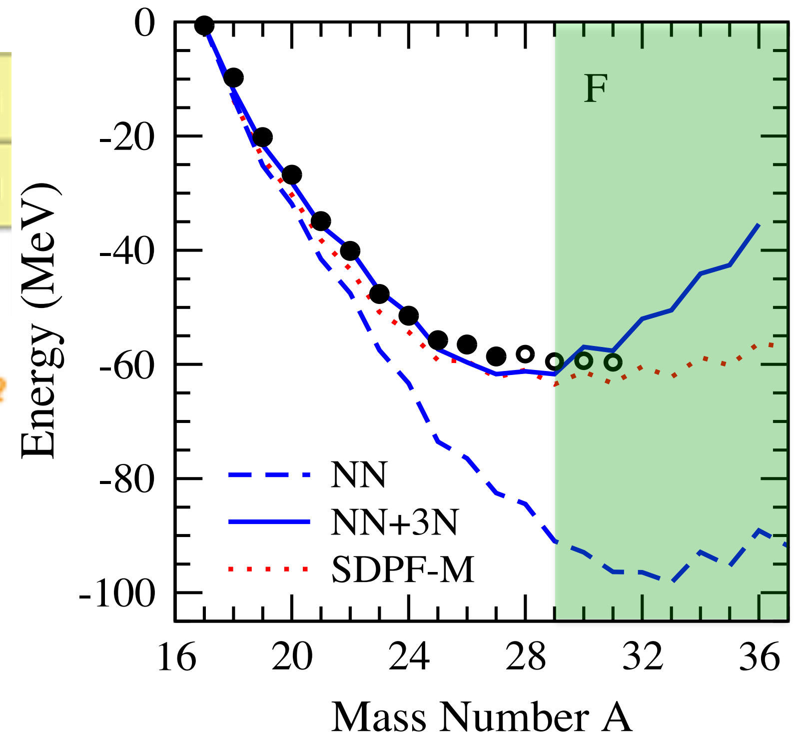

JDH, Menendez, Schwenk, in prep.

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**

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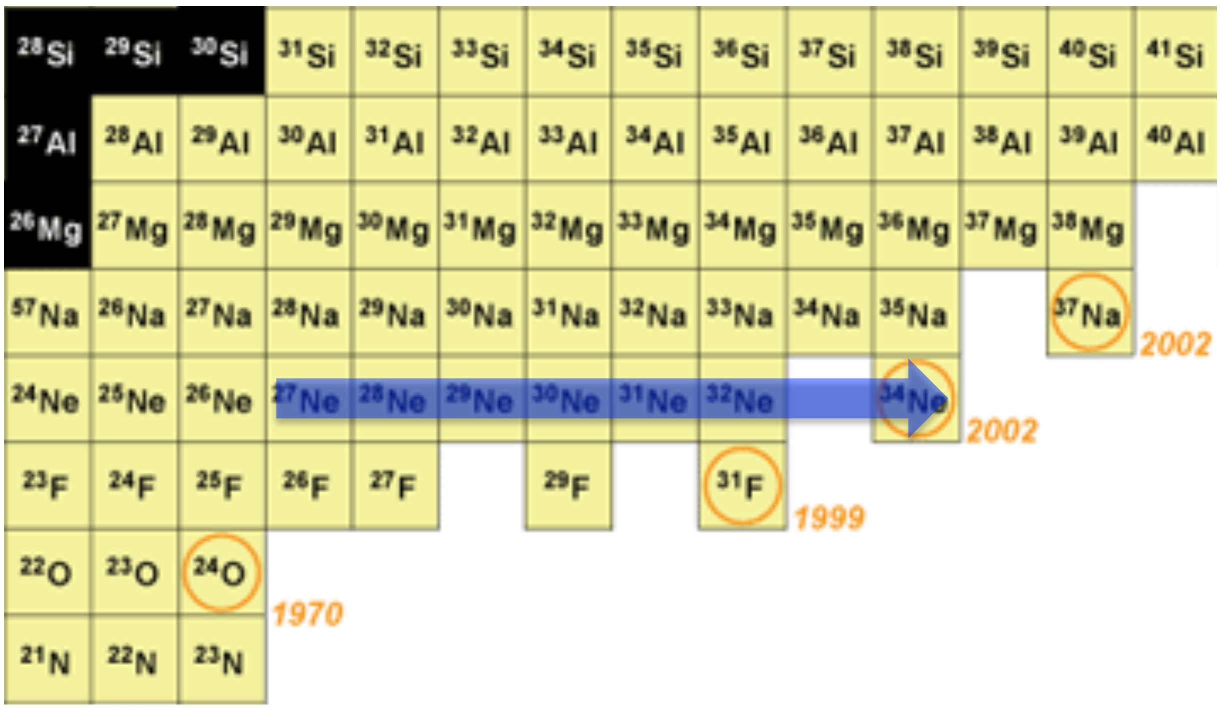
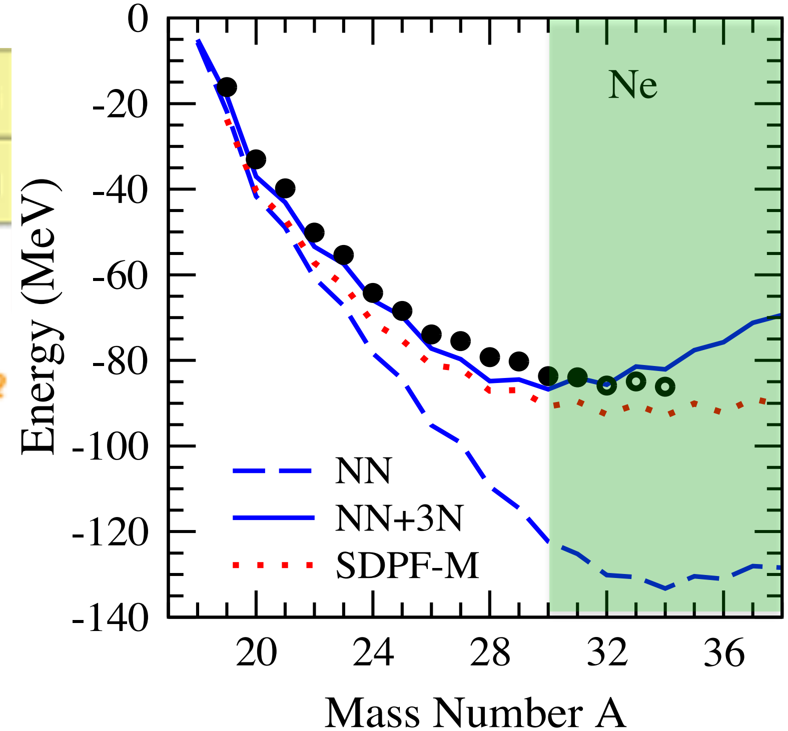




JDH, Menendez, Schwenk, in prep.

Similar behavior in Neon isotopes

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

Tsunoda, Hjorth-Jensen, Otsuka

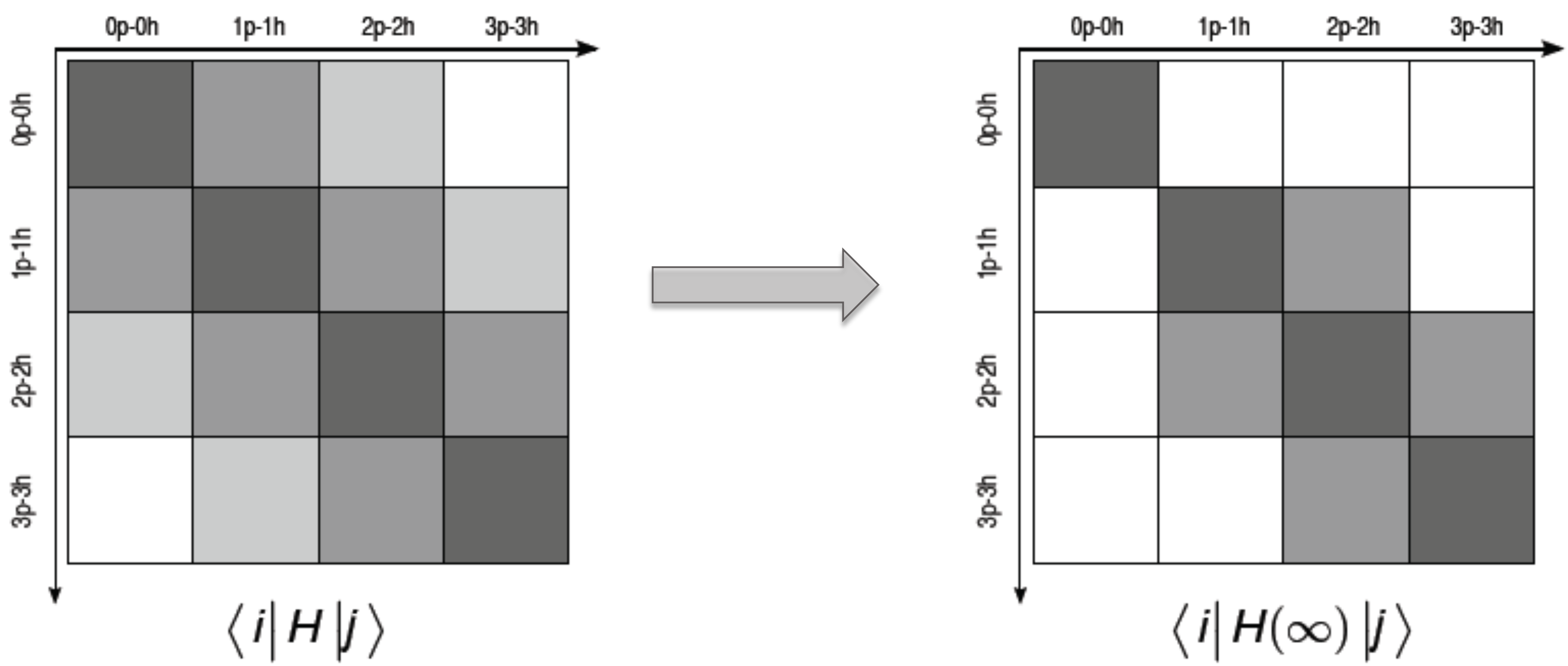
IM-SRG for Valence-Space Hamiltonians

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



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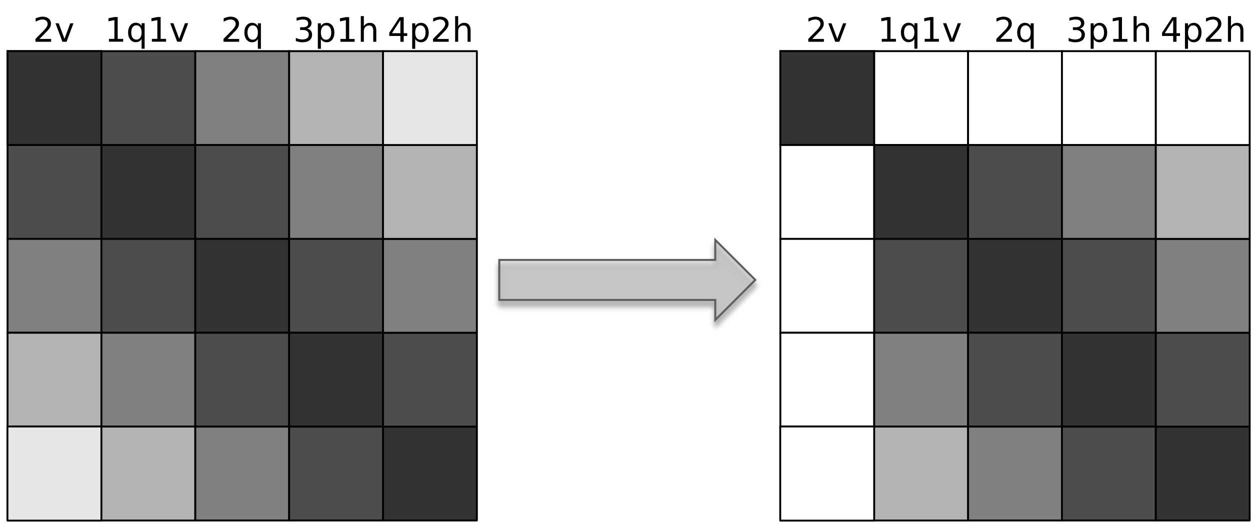
Tsukiyama, Bogner, Schwenk, PRC (2012)

Open shell systems:

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

Redefine "off-diagonal" to exclude valence particles



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

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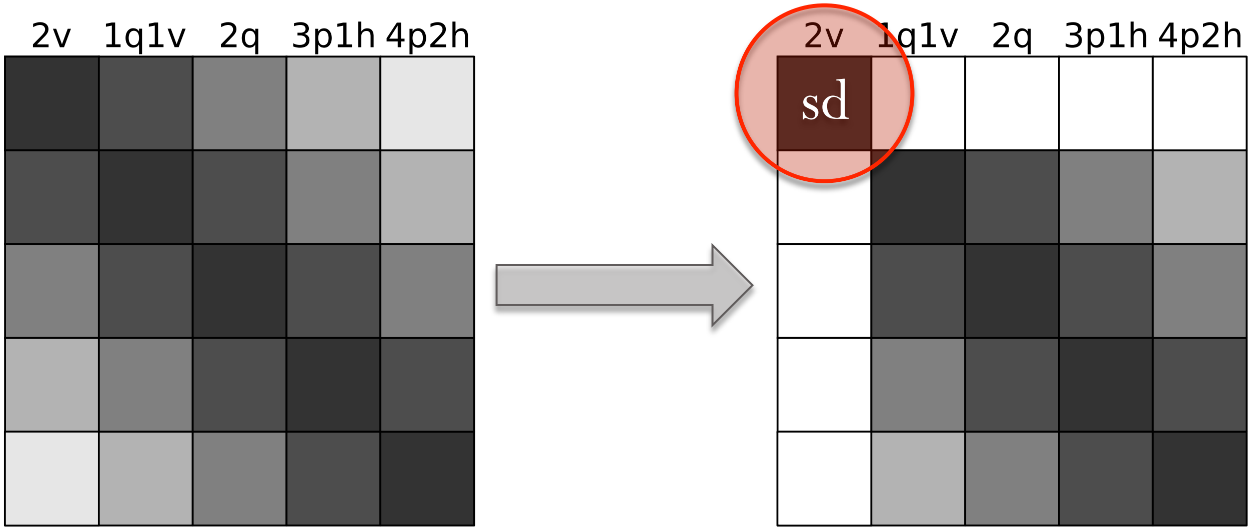


$$H(s=0) \rightarrow H(\infty)$$

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 $e_{\text{max}} = 2n + l = 14$ **converged**

★4) NN and 3N forces from chiral EFT

5) Explore extended valence spaces – in progress

NN matrix elements

- Chiral N^3LO (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

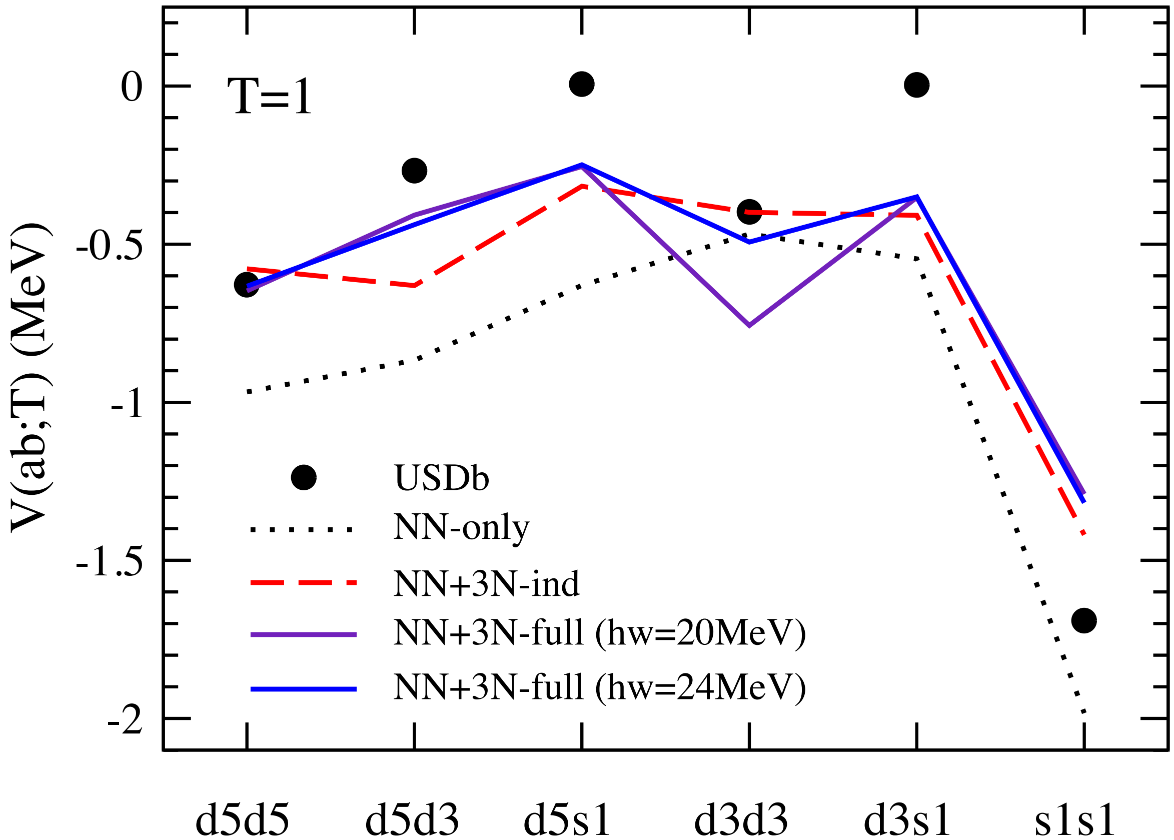
Initial 3N force contributions

- Chiral N^2LO $\Lambda_{3N} = 400\text{MeV}$
- Included with cut: $e_1 + e_2 + e_3 \le E_{3\,\text{max}} = 14$

IM-SRG Monopoles

Monopoles: angular average of interaction

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



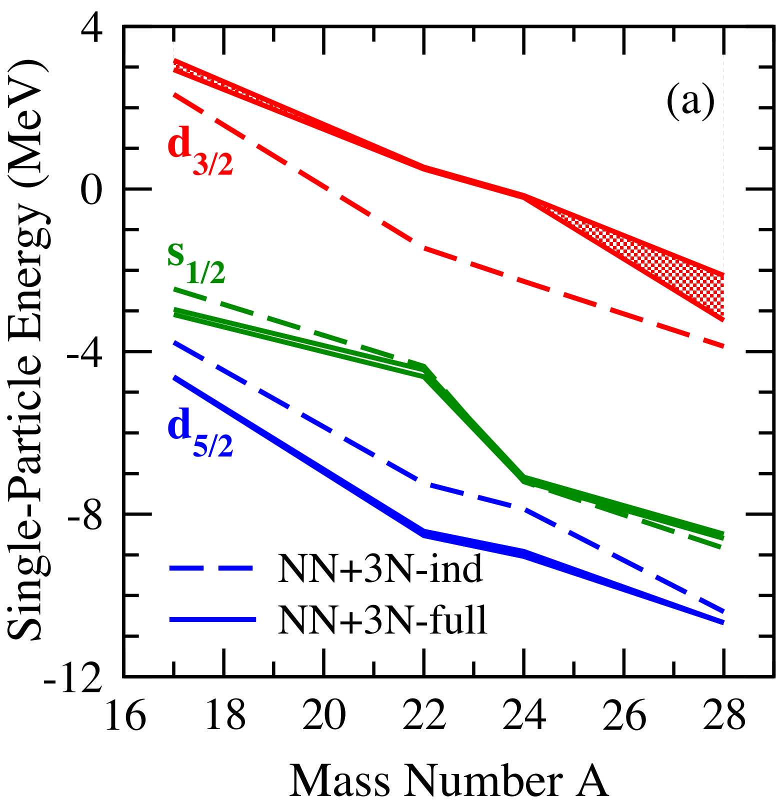
$$V_{ab}^{T} = \frac{\sum_J (2J+1)\ V_{abab}^{JT}}{\sum_J (2J+1)}$$

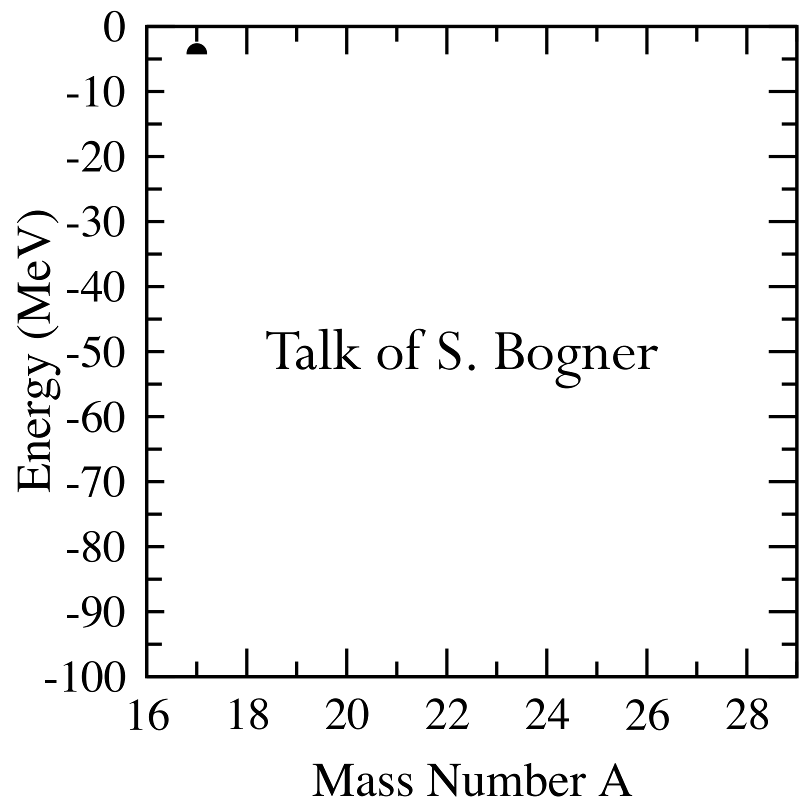
NN-only too attractive

NN+3N-full similar trend to USDb

IM-SRG Oxygen Ground-State Energies

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





Bogner et al., arXiv: 1402.1407

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

Good dripline properties?

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!

Acknowledgments

Collaborators

J. Menendez J. Simonis A. Schwenk
S. Binder, A. Calci, J. Langhammer, R. Roth

S. Bogner **H. Hergert**

T. Otsuka T. Suzuki (Nihon U.)