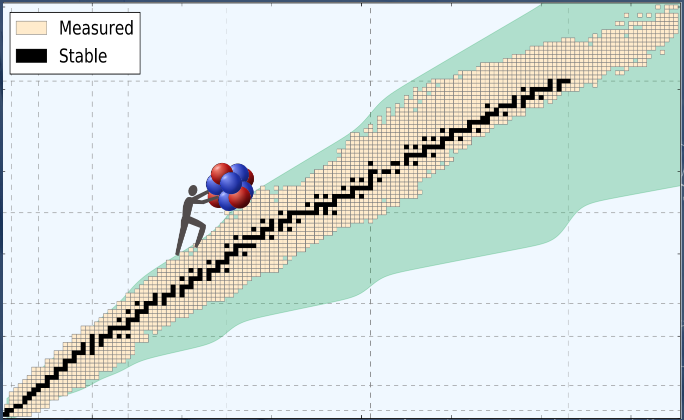
TRIUMF

Canada's national laboratory
for particle and nuclear physics
and accelerator-based science

Extending the reach of ab initio theory: Valence space IMSRG

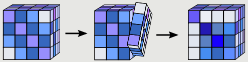


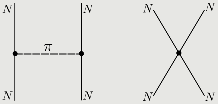
Ragnar Stroberg

TRIUMF

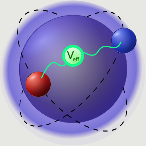
ARIS In the Mountains
Keystone, Colorado
May 30, 2017

Outline





1. In-medium SRG for a valence space
2. Ensemble normal ordering
3. Selected results
4. Outlook



Work in collaboration with: A. Calci, J. Holt, P. Navrátil, S. Bogner, H. Hergert, N. Parzuchowski, K. Hebeler, R. Roth, A. Schwenk, J. Simonis, C. Stumpf, G. Hagen, and T. Morris

- $H|\Psi\rangle = E|\Psi\rangle$ is too dif
- Perform unitary transfor (implicit change of basis solve.

$$H|\Psi\rangle = E|\Psi\rangle$$

complicated!

- Iterative/guess-and-check approach.

$$U \equiv e^{\Omega} = e^{\Omega_n} e^{\Omega_{n-1}} \dots e^{\Omega_2} e^{\Omega_1}$$

- Alternatively, $\Omega_n \rightarrow \eta ds \Rightarrow$ flow equation
- Computational effort dominated by commutator evaluation.

Głazek and Wilson PRD (1994), Wegner (1994), Bogner, Furnstahl, and Perry (2007), Morris et al (2015)

Similarity renormalization group (SRG)

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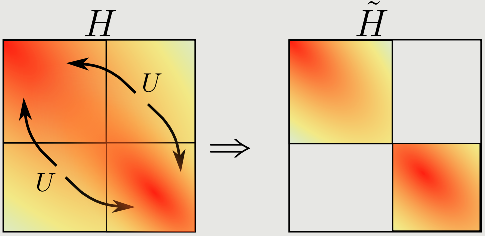
- Perform unitary transformation $\tilde{H} = UHU^\dagger$ (implicit change of basis) so SE is easier to solve.



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$$\frac{dH(s)}{ds} = [\eta(s), H(s)].$$

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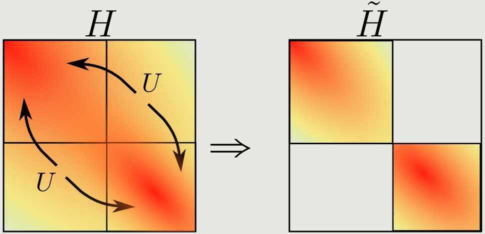

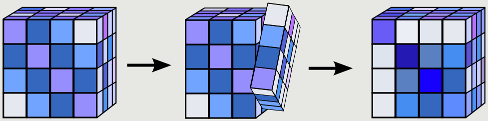

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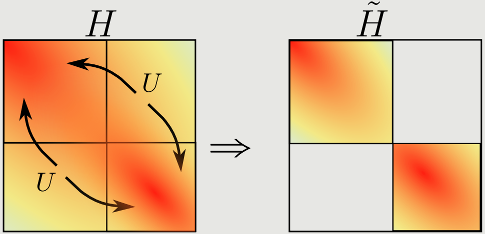

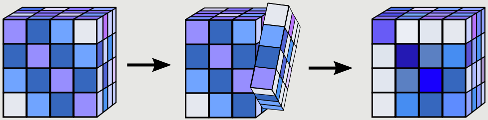

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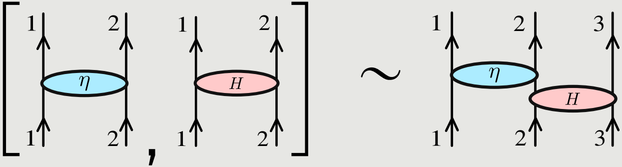
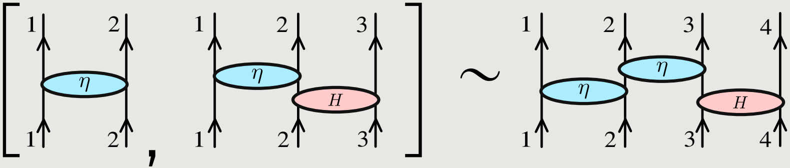
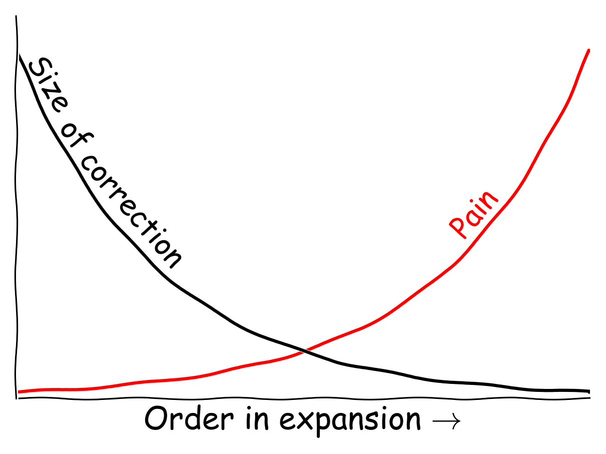


(Two-body) (Two-body) (Three-body)



(Two-body) (Three-body) (Four-body)

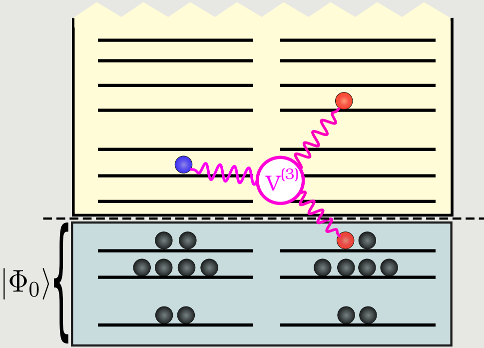
What we would like:



Why "in-medium"?

$$H = \underbrace{E_0}_{\text{0-body}} + \underbrace{\sum_{ij} H_{ij}\{a_i^\dagger a_j\}}_{\text{1-body}} + \underbrace{\frac{1}{4}\sum_{ijkl} H_{ijkl}\{a_i^\dagger a_j^\dagger a_l a_k\}}_{\text{2-body}} + \underbrace{\frac{1}{36}\sum_{ijklmn} H_{ijklmn}\{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}}_{\text{3-body}} + \dots$$

- In general, the transformation U will induce 4-body, 5-body, etc. forces
- Write H in terms of excitations out of reference $|\Phi_0\rangle$
- Normal ordering: $\langle\Phi_0|\{a_1^\dagger \dots a_N^\dagger a_N \dots a_1\}|\Phi_0\rangle = 0$
- If $|\Phi_0\rangle \approx |\Psi\rangle$, higher-body terms are negligible
- **Truncate all operators at 2 body level (NO2B)**



Tskukiyama et al (2011)

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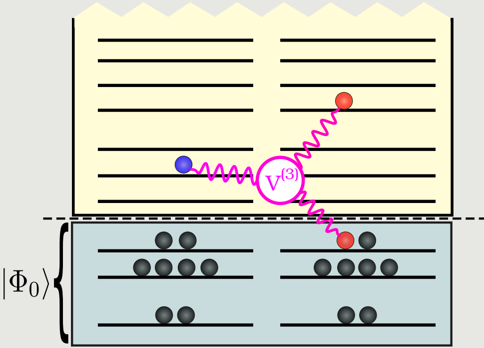

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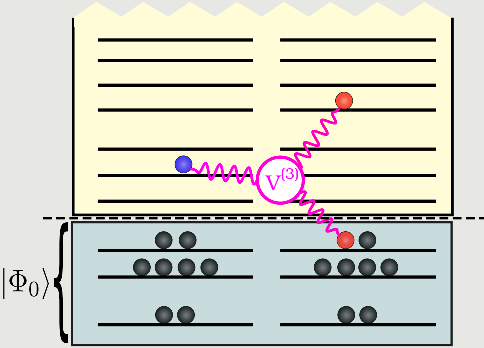
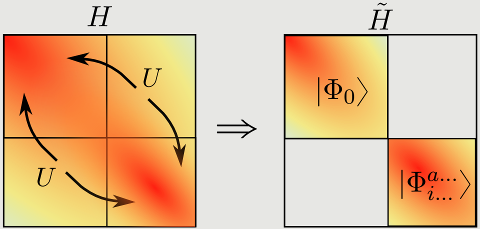
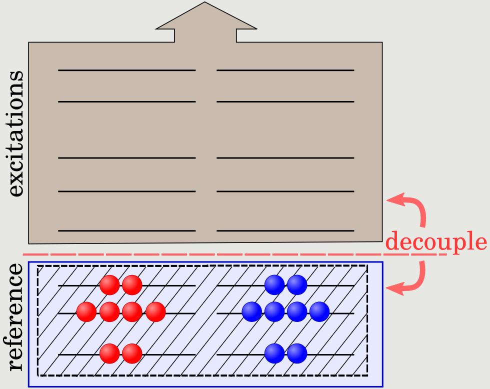


Tskukiyama et al (2011)

Solving the many-body problem

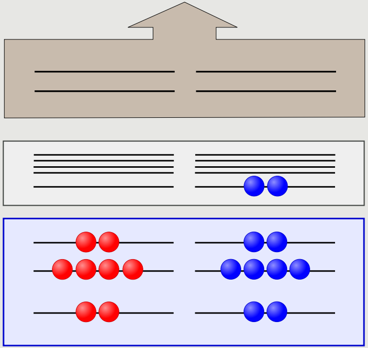




- Decouple a 1×1 sub-block
- Use SRG to suppress excitations out of $|\Phi_0\rangle$
- After decoupling, energy is $E_0 = \langle\Phi_0|\tilde{H}|\Phi_0\rangle$

Open shell systems

- Open shell systems: multiple (quasi-) degenerate configurations $\Rightarrow$ strong mixing, $|\Phi_0\rangle \not\approx |\Psi\rangle$
- Single Slater determinant may not have good total angular momentum J
- Large rotation angle $\Rightarrow$ induced many-body forces
- Strategies:
  - Break symmetries and restore afterward
  - Construct multi-configuration reference, then decouple (multi-reference IM-SRG)
  - Decouple a subset of configurations, then construct state from them using standard shell model machinery, e.g NuShellX (valence-space IMSRG)



Tsukiyama et al. (2012), Hergert et al. (2013), Bogner et al. (2014)

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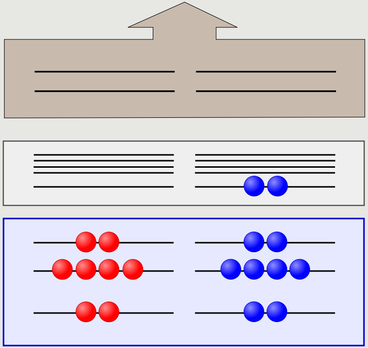

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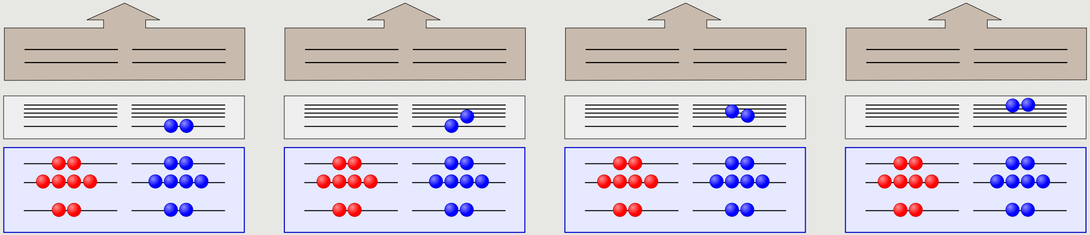
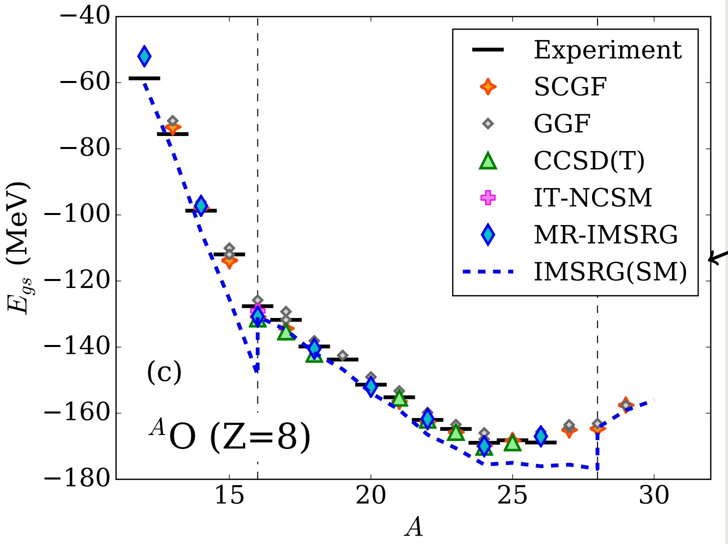
What reference should be used when decoupling a valence space?

(i.e. what is the "medium"?)



Obvious choice: the inert core, e.g. ^{16}O.

Ensemble normal ordering



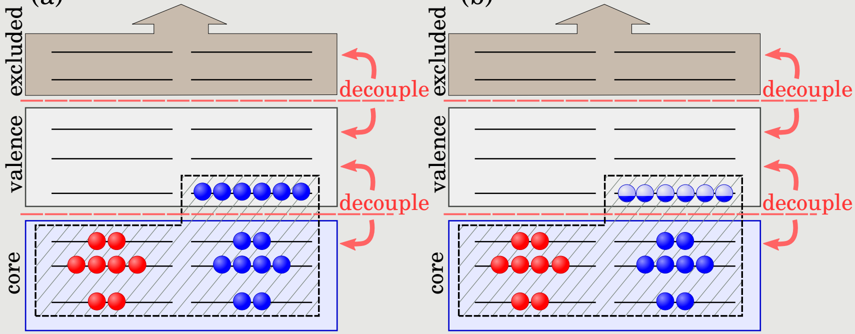
Reference: inert core

Somà et al. PRC (2013), Cipollone et al. PRC (2015), Jansen et al. PRL (2014), Roth et al. PRL (2012), Hergert et al. PRL (2013), Bogner et al. PRL (2014)

Ensemble normal ordering

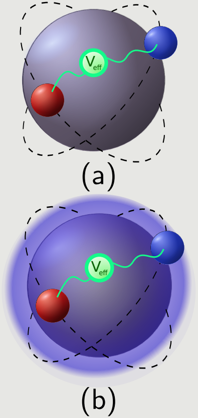
$$\langle \Phi_0 | \{a_i^\dagger \dots a_N\} | \Phi_0 \rangle = 0$$

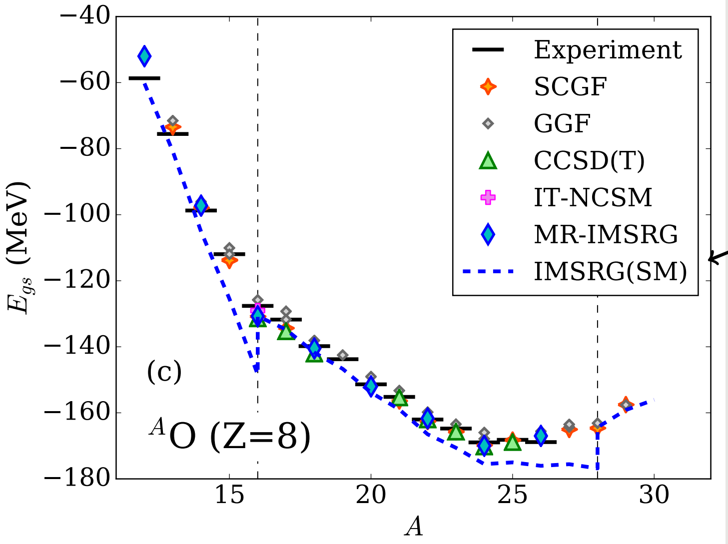
$$\mathrm{Tr}\left(\rho \{a_i^\dagger \dots a_N\}\right) = 0$$



$$|\Phi_0\rangle = |^{22}\mathrm{O}\rangle$$

$$\rho = \sum_\alpha c_\alpha |\Phi_\alpha\rangle\langle\Phi_\alpha|$$





Reference:
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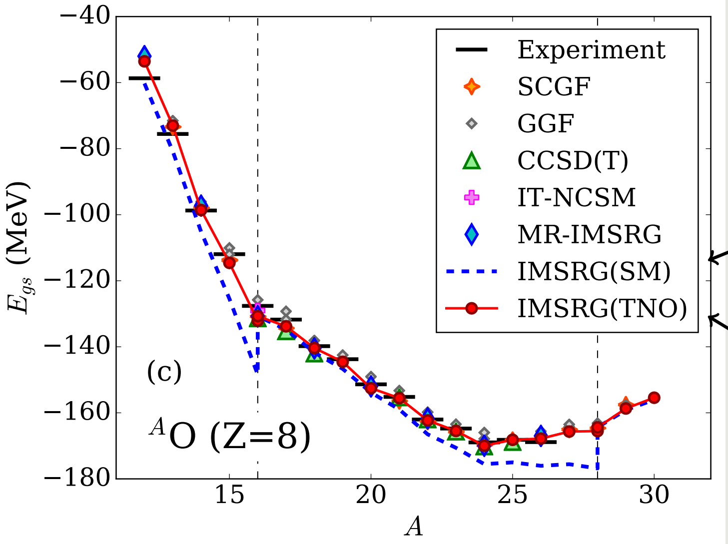
Ensemble normal ordering

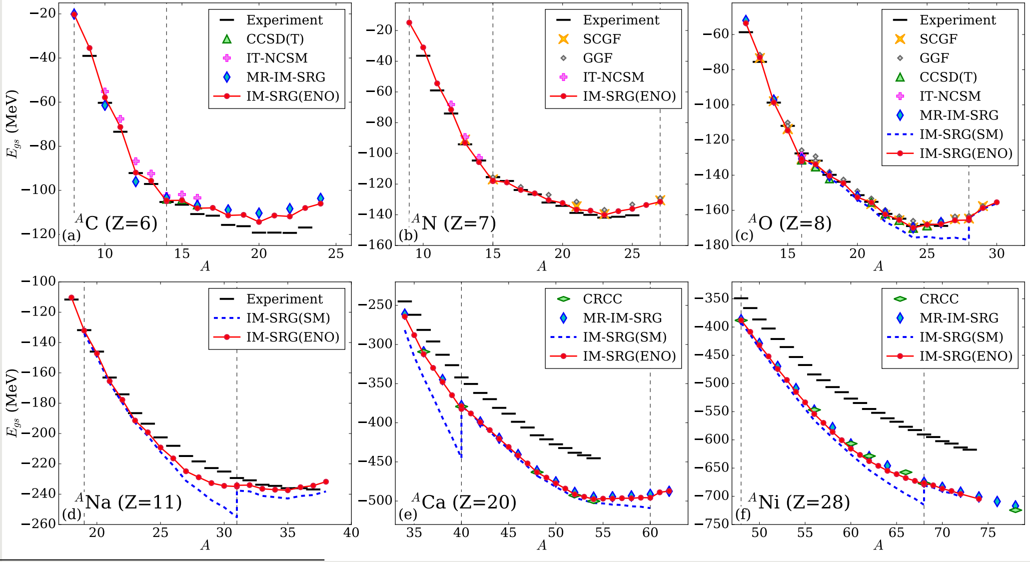


Reference: inert core

Reference: nearest closed shell

(Ensemble gives very similar results)

Ground state energies



SRS et al. PRL (2017)

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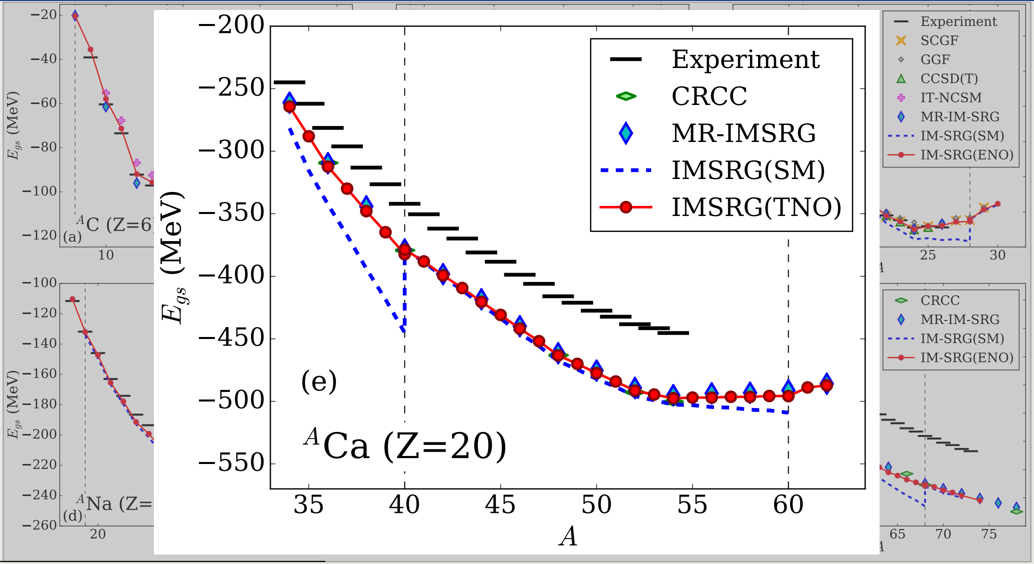
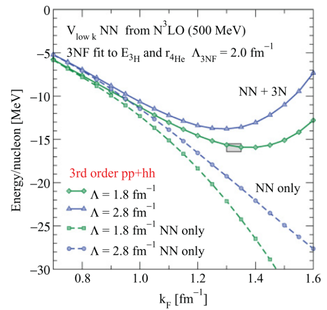


SRS et al. PRL (2017)

	EM 500/400	EM 1.8/2.0
NN	N^{3}LO $\Lambda_{2N} = 500$ MeV non-local regulator fit to NN scattering, ^{2}H $\lambda_{SRG} = 1.88$ fm^{-1}	same same same same $\approx$ same
3N	N^{2}LO $\Lambda_{3N} = 400$ MeV **local regulator** **fit to ^{3}H BE, $t_{1/2}$** **consistently SRG evolved**	same $\approx$ same **non-local regulator** **fit to ^{3}H BE, ^{4}He r_{ch}** **no SRG for 3N**



Entem and Machleidt PRC (2003), Gazit et al PRL (2009), Hebeler et al. PRC(R) (2011), Drischler et al. PRC (2016), Simonis et al. arxiv:1704.02915

Saturation and finite nuclei

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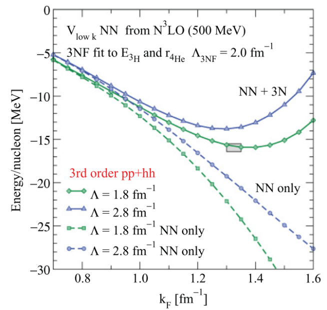

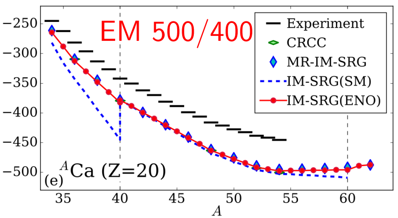

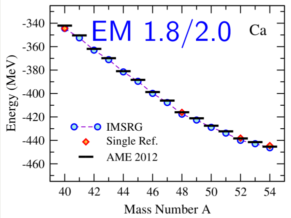

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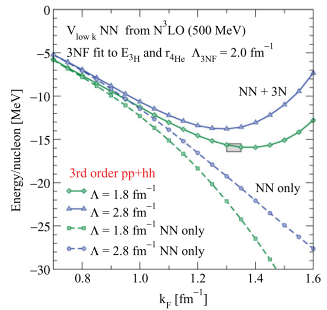
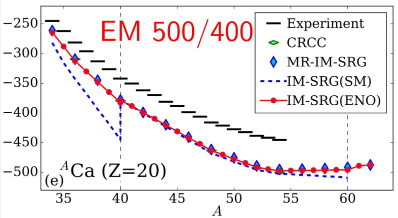
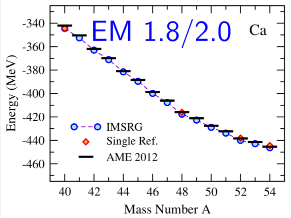






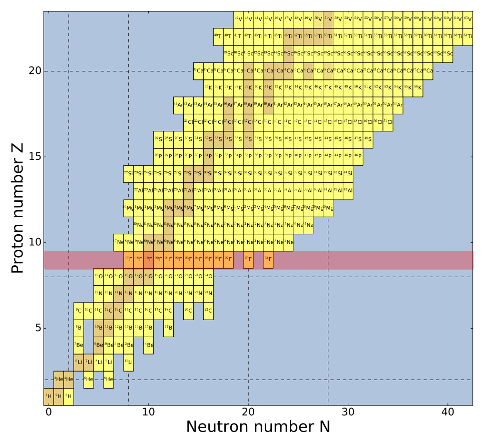
- Neither interaction is fully consistent

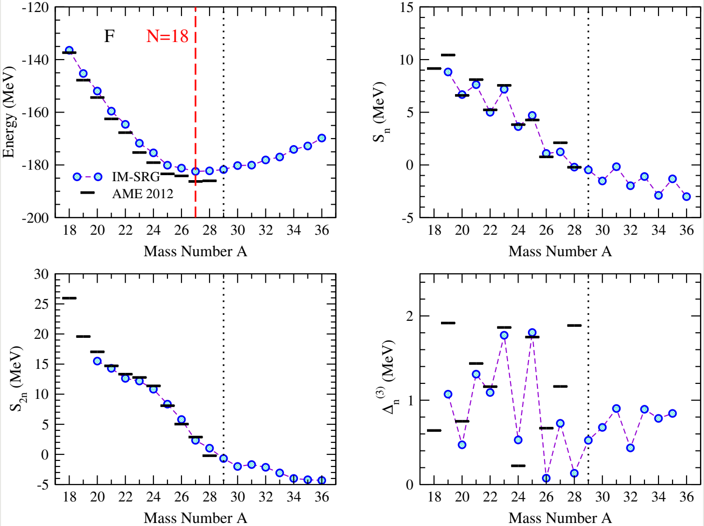
  however…

- Saturation properties are important for finite nuclei

Entem and Machleidt PRC (2003), Gazit et al PRL (2009), Hebeler et al. PRC(R) (2011), Drischler et al. PRC (2016), Simonis et al. arxiv:1704.02915

EM 1.8/2.0 interaction





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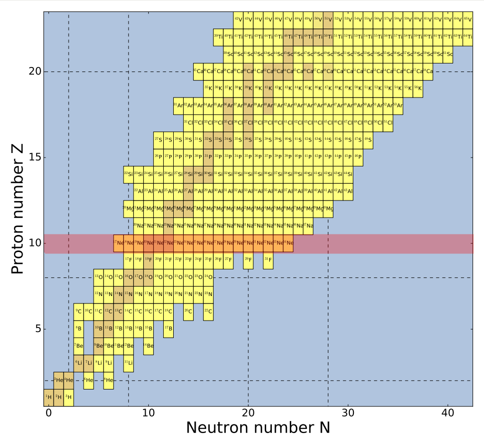

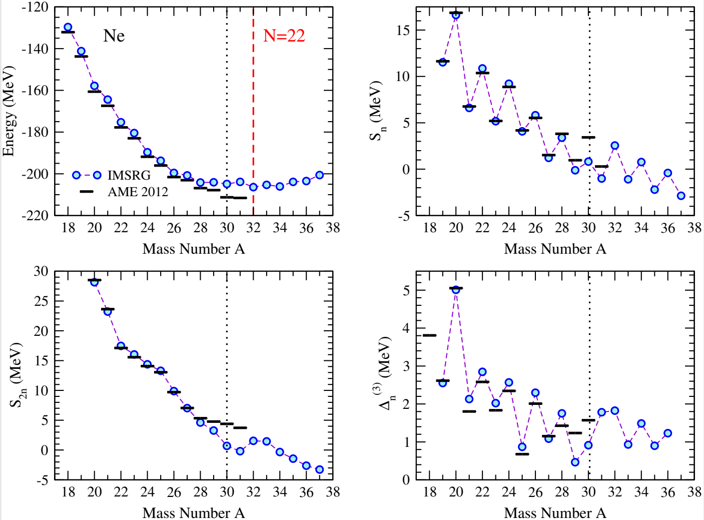

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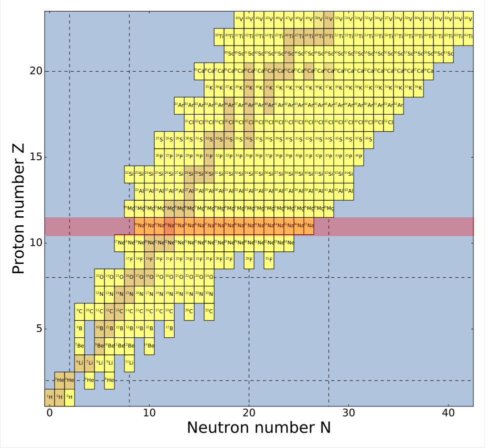

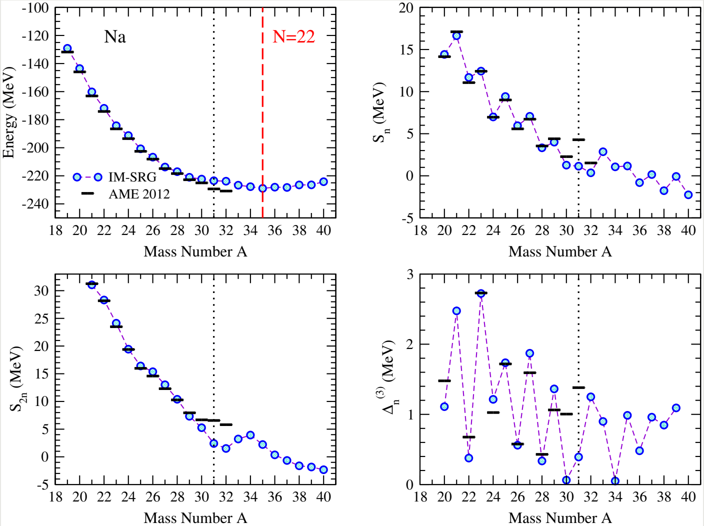

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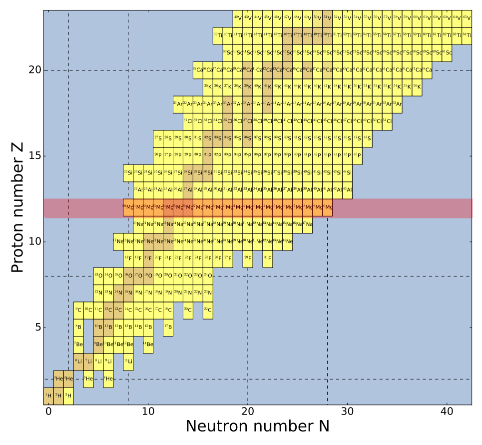

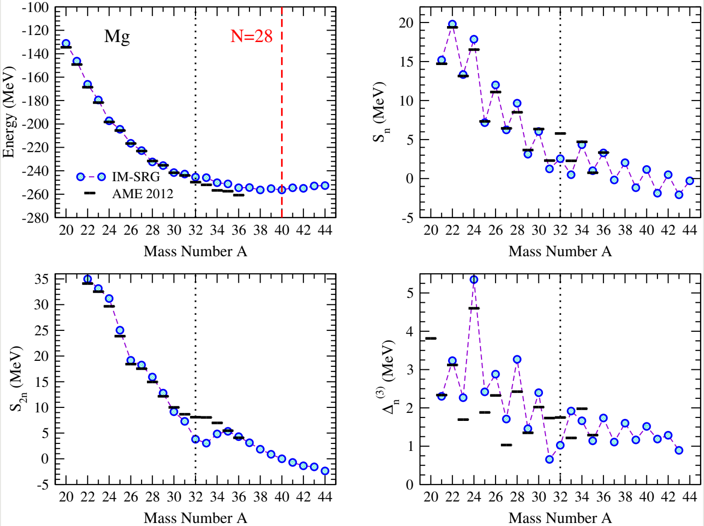

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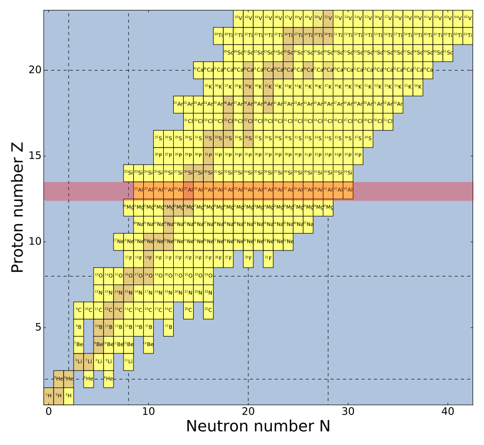

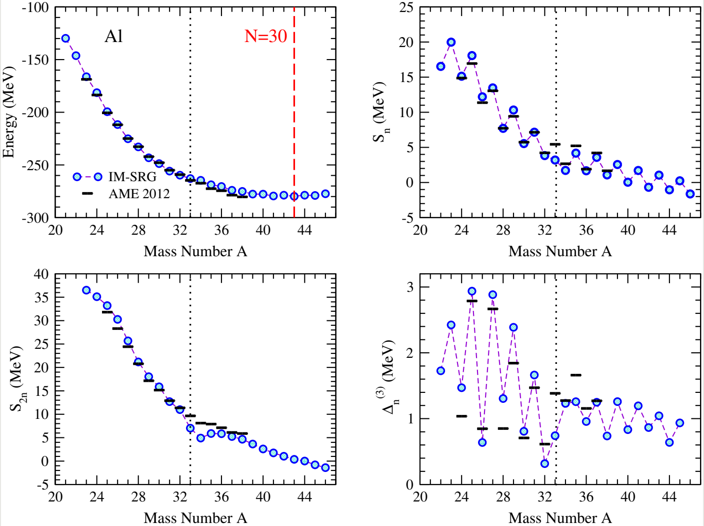

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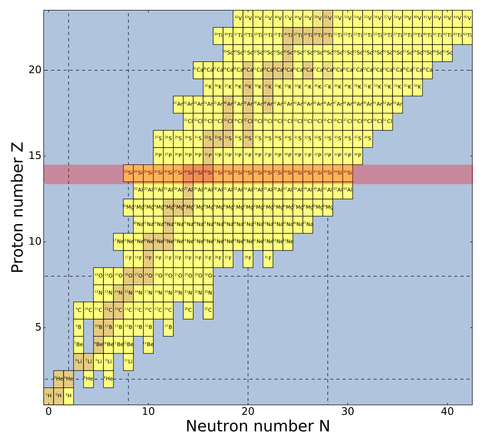

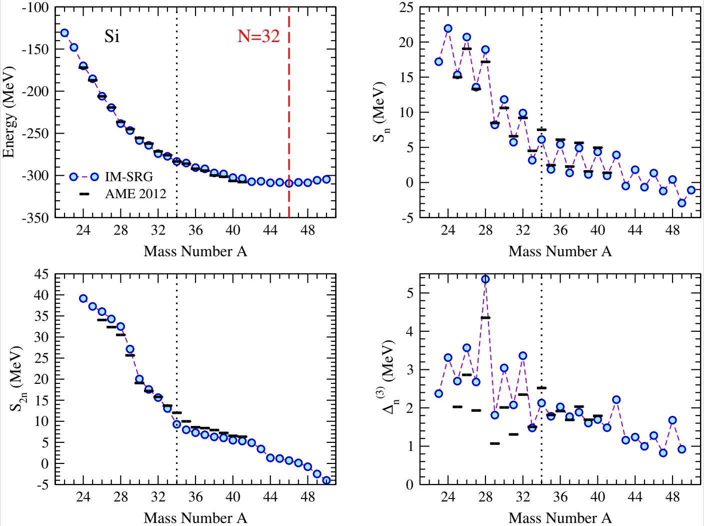

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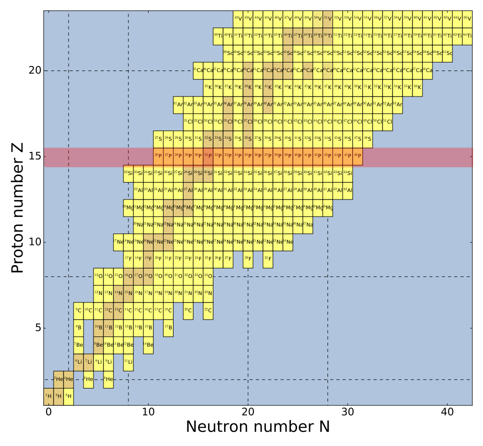

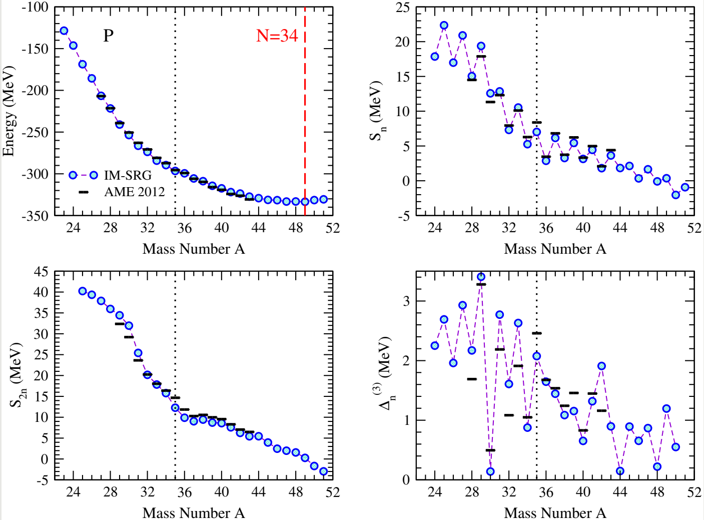

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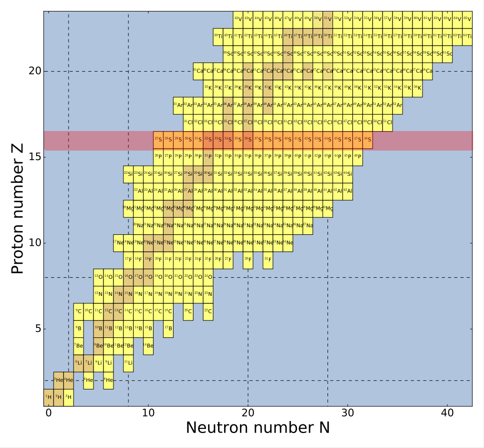

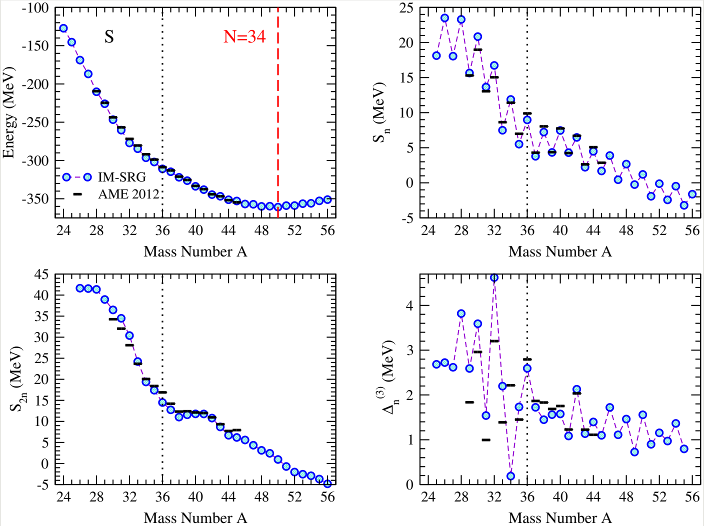

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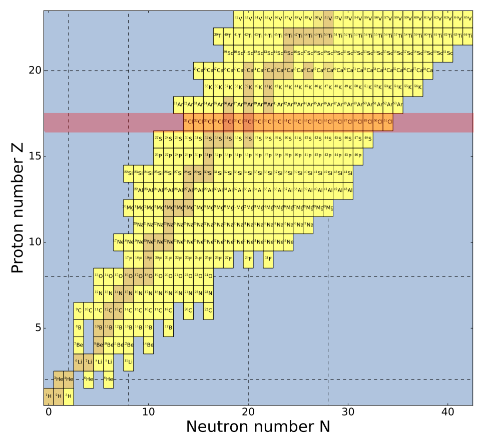

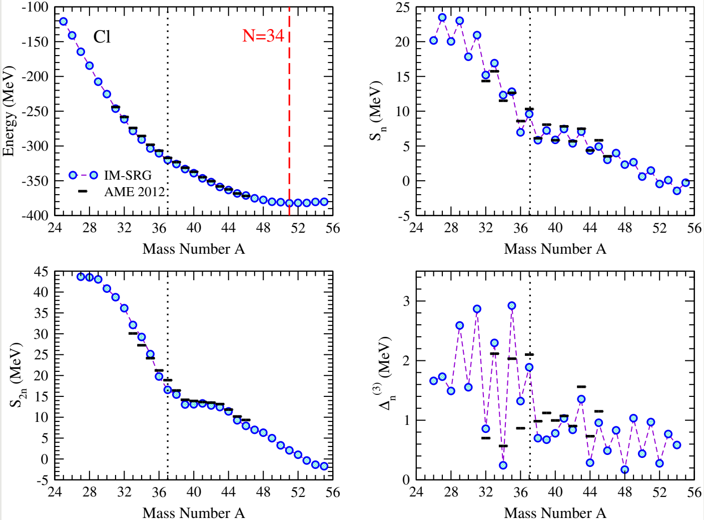

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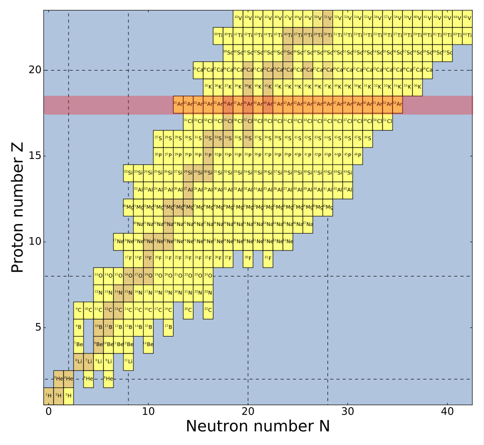

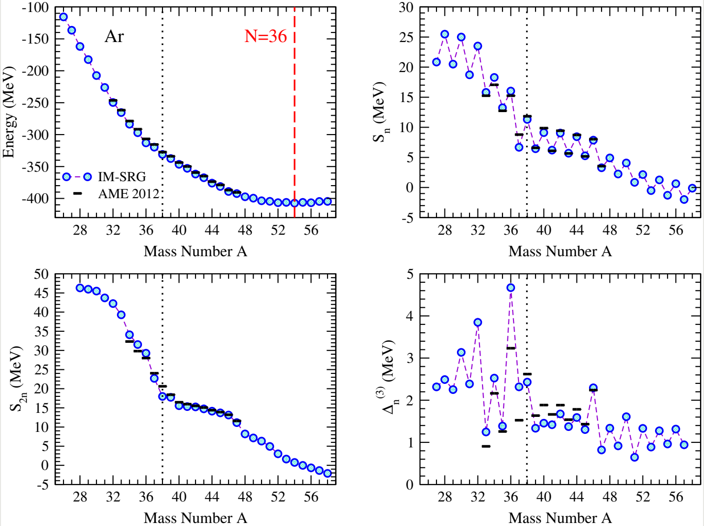

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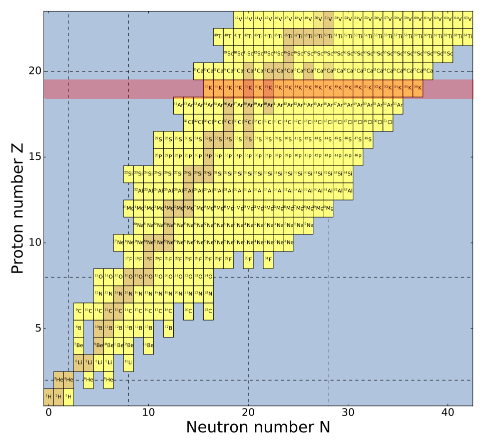
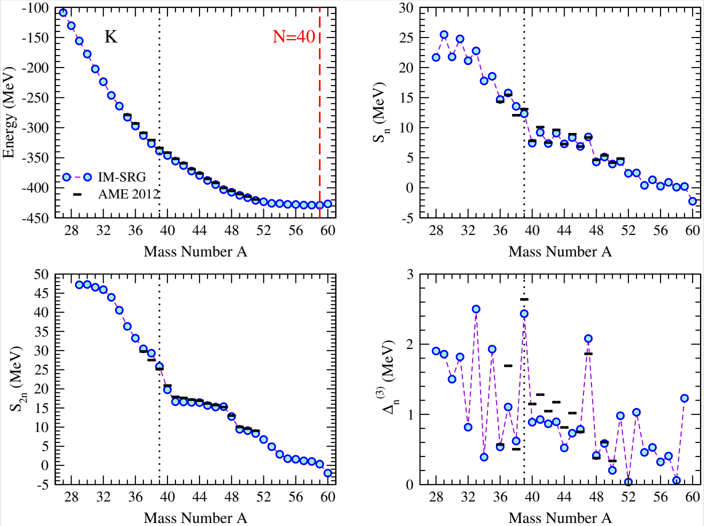
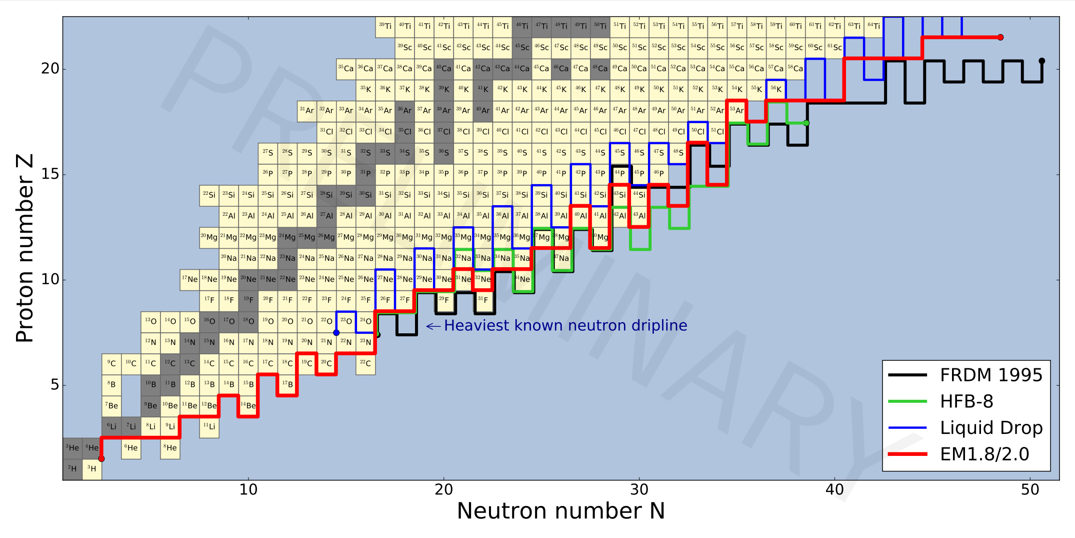


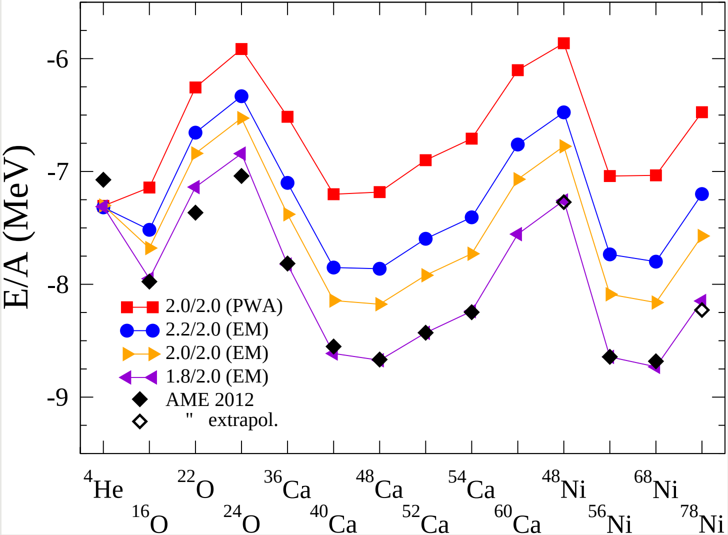




Baumann et al. Nature (2007), Möller et al. (1995), Samyn et al. (2004), Holt et al. (in prep.)

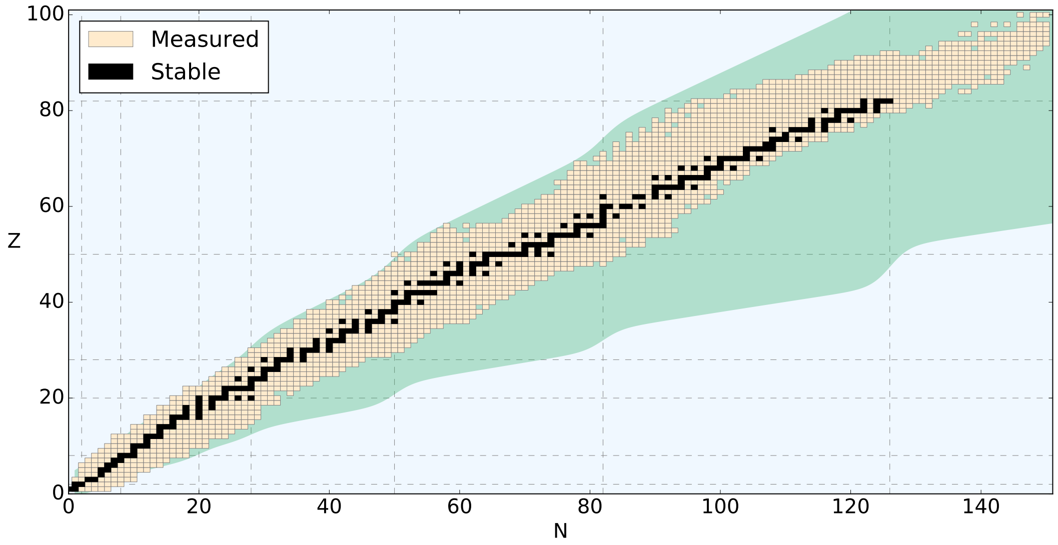
A note of caution

- Only difference: choice of initial NN force.
- Identical procedure for fitting 3N contact terms.
- Based on few-body data, all interactions are equally good.
- Big differences for finite nuclei.
- 1.8/2.0 EM interaction is "magic", i.e. lucky.



Simonis et al. arxiv:1704.02915

The reach of ab initio theory



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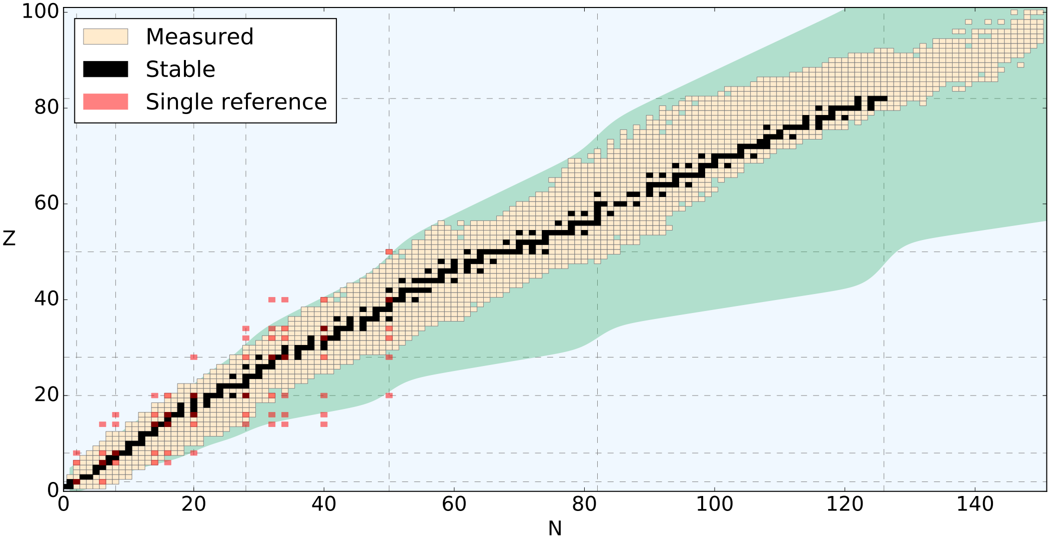

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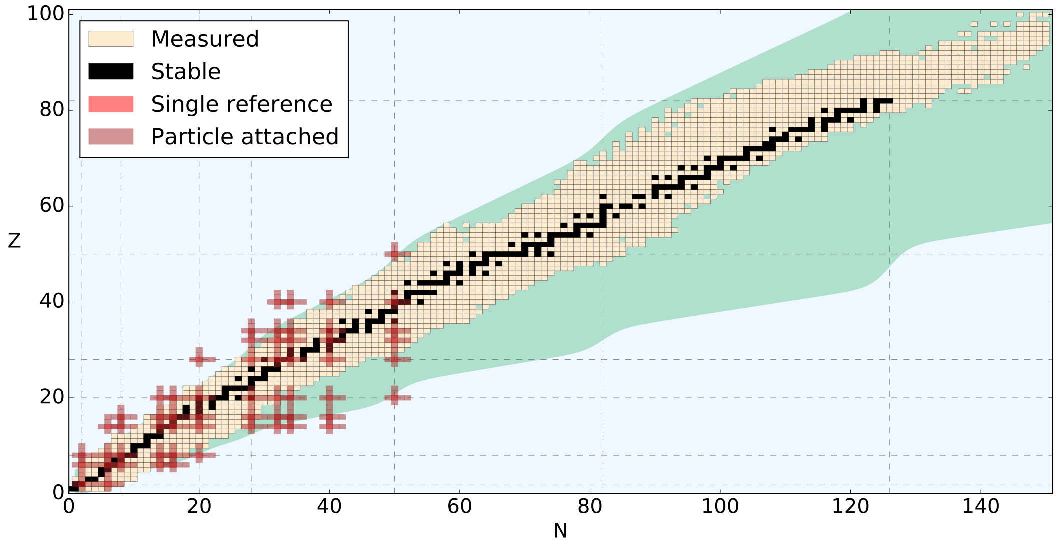

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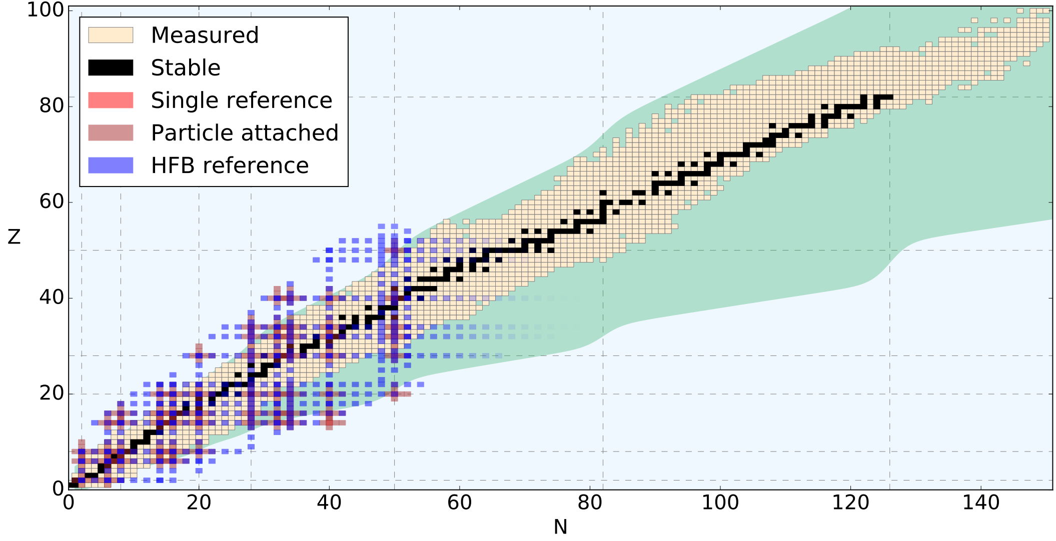

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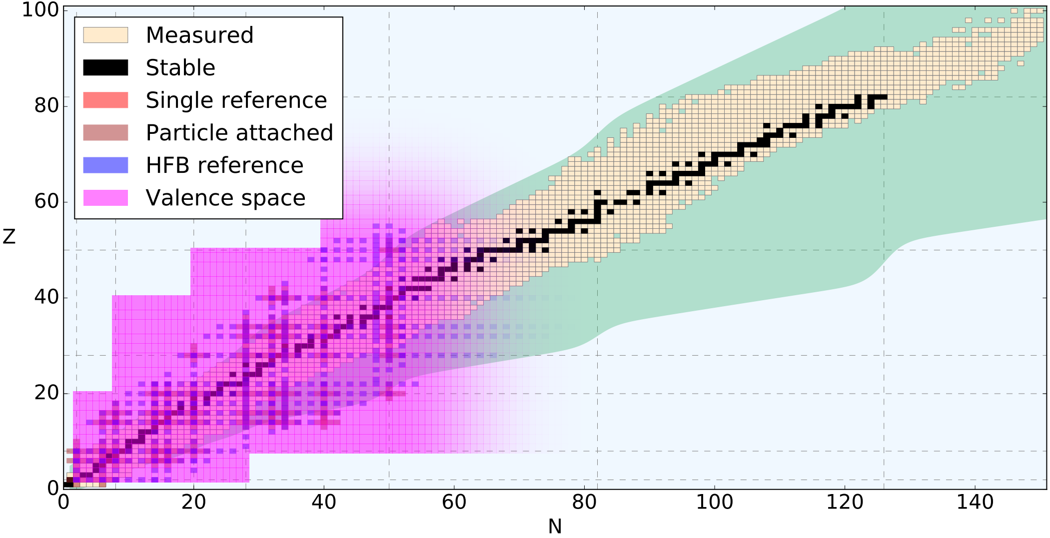
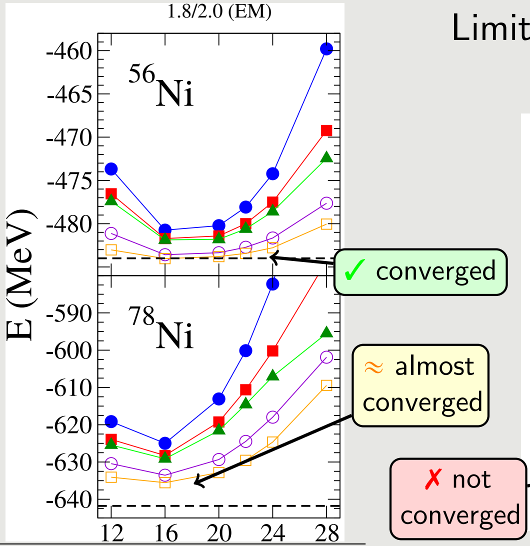
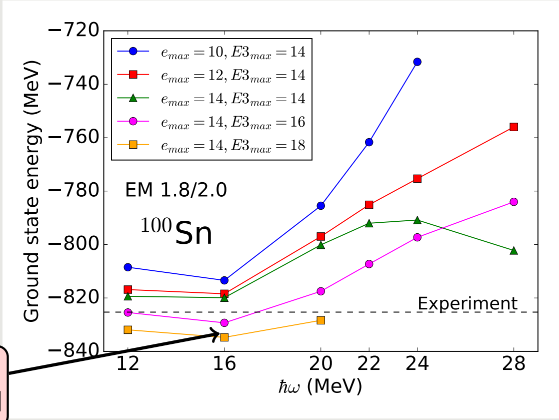


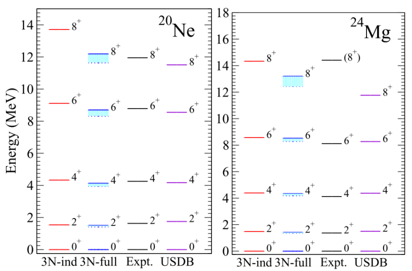


Simonis et al. arXiv:1704.02915 (2017)

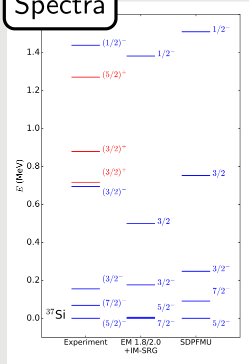
Limited by truncation of 3N matrix elements

$$E3_{max} = e_1 + e_2 + e_3$$



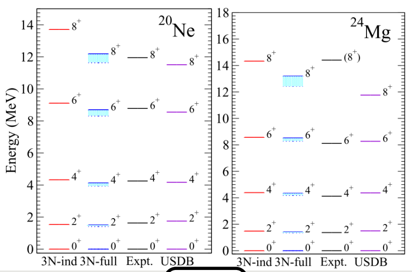


Spectra



Bogner et al. PRL (2014), SRS et al. PRC(R) (2016),

Beyond binding energies



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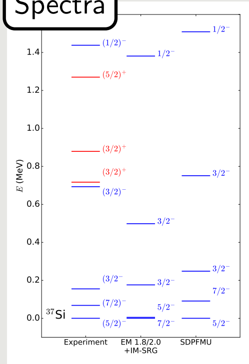
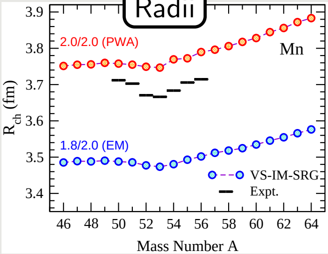


Radii



Bogner et al. PRL (2014), SRS et al. PRC(R) (2016), Simonis et al arXiv:1704.02915 (2017),

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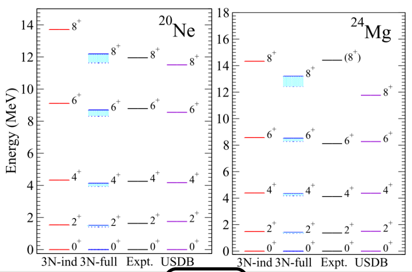
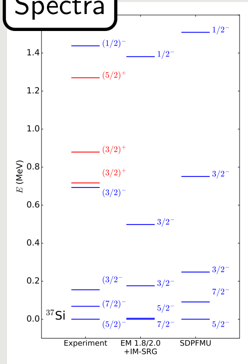


Spectra



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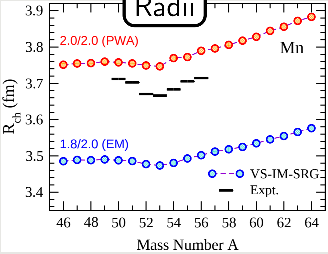
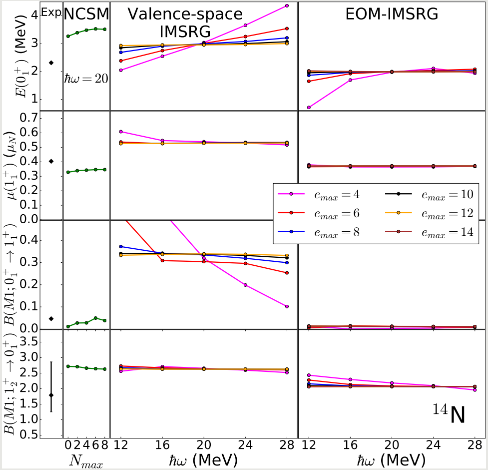


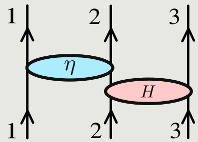
Electroweak Observables



Bogner et al. PRL (2014), SRS et al. PRC(R) (2016), Simonis et al arXiv:1704.02915 (2017), Parzuchowski et al. arXiv:1705.05511 (2017)

What does the future hold?
(Technical developments)

- Quantification of many-body uncertainty
  - Perturbative estimation of omitted 3-body terms
  - Invariant trace
  - Full IMSRG(3): Include 3-body terms throughout the calculation



- Heavy-mass frontier
  - Improve handling of 3N forces
- Decoupling arbitrary valence spaces
  - Island(s) of inversion
  - Parity-changing transitions, e.g. $E1$
- Improved basis
  - Two-frequency oscillator basis for halo systems
  - Explicit inclusion of collective modes

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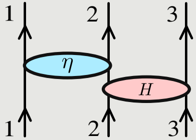

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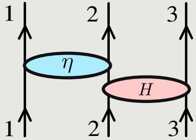

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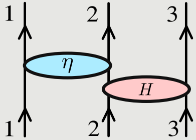

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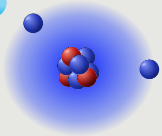
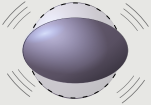
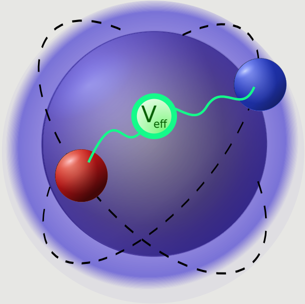




What does the future hold? (Observables)

- Radii / isotope shifts
- $E0$ transitions
- Chiral currents for $M1$, Gamow-Teller operators
- Neutrinoless double beta decay
- Structure factors for dark matter detection
- Superallowed Fermi decays
- Suggestions?

- Valence space IM-SRG with ensemble normal ordering allows access to all nuclei up to A~ 100
- Reach in A is presently limited by E_{3max} truncation
- Consistent operators for other observables can be obtained
- Chiral interactions still need work (magic notwithstanding)
- Next goal: how to reliably estimate truncation error?



Collaborators:

TRIUMF A. Calci, J. Holt, P. Navrátil, C. Payne, O. Drozdowski, D. Fullerton, C. Gwak, L. Kemmler, S. Leutheusser, D. Livermore

NSCL/MSU S. Bogner, H. Hergert, N. Parzuchowski

TU Darmstadt K. Hebeler, R. Roth, A. Schwenk, J. Simonis, C. Stumpf

ORNL/UT G. Hagen, T. Morris