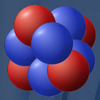
Canada's national laboratory
for particle and nuclear physics
and accelerator-based science

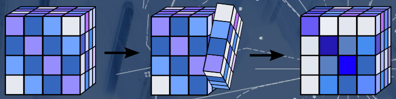
# In-medium SRG for fully open-shell systems

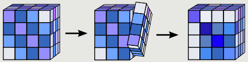

Ragnar Stroberg

TRIUMF

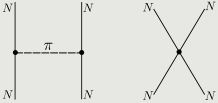

Ab initio workshop
TRIUMF
March 2, 2017



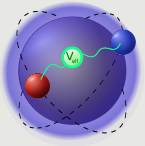




# Outline




1. In-medium SRG
2. Ensemble normal ordering
3. Non-standard valence spaces

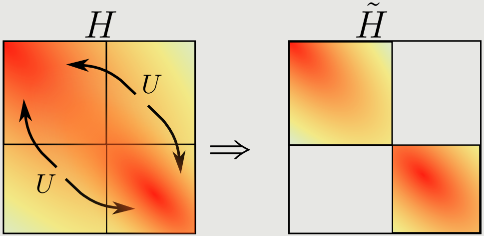


# Similarity renormalization group (SRG)

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




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

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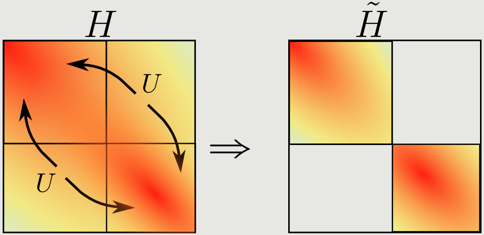


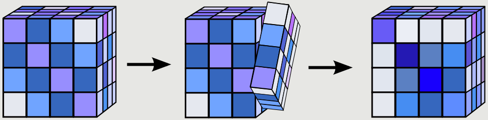

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$$\frac{dH(s)}{ds} = [\eta(s), H(s)].$$

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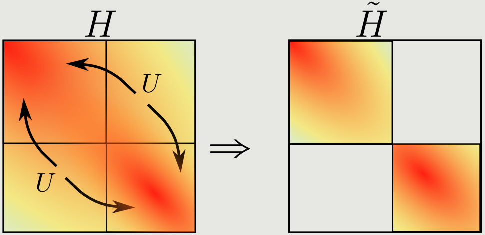


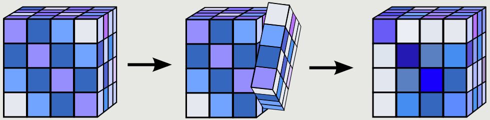

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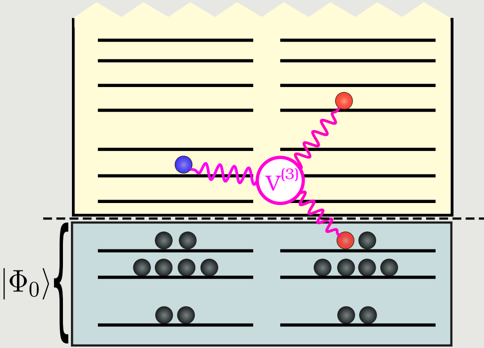
# Why "in-medium"?

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

- In general, the transformation $U$ will induce 4-body, 5-body, etc. forces
- Write $H$ in normal-ordered form w.r.t reference $|\Phi_0\rangle$
- $\langle\Phi_0|\{a_1^\dagger \ldots a_N^\dagger a_N \ldots a_1\}|\Phi_0\rangle = 0$
- If $|\Phi_0\rangle \approx |\Psi\rangle$, higher-body terms are negligible
- **Truncate all operators at 2 body level**




Tskukiyama et al (2011)

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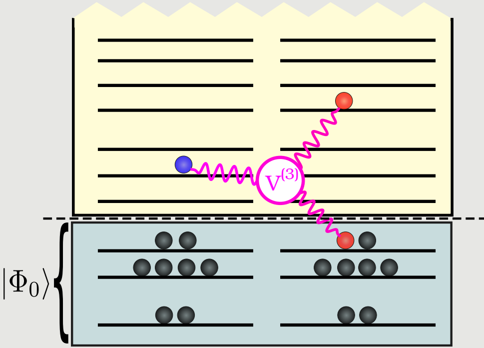


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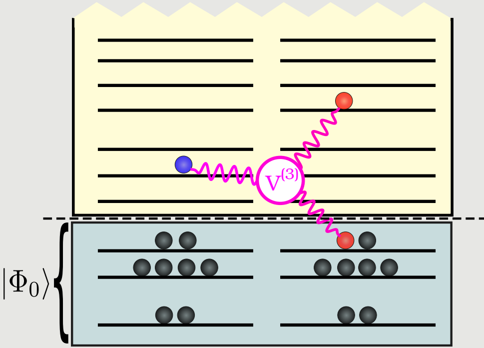


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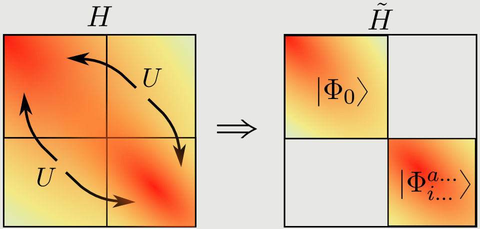
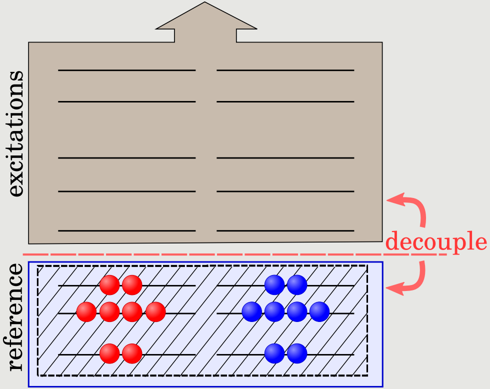
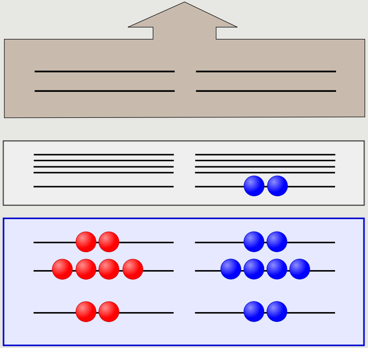
## Solving the many-body problem




- Decouple a $1\times 1$ 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: multiple (quasi-) degenerate configurations. $|\Phi_0\rangle \not\approx |\Psi\rangle$
- 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-determinant reference, then decouple (multi-reference IM-SRG)
  - Decouple a subset of determinants, then construct state from them (valence-space IMSRG)



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

# Open shell systems

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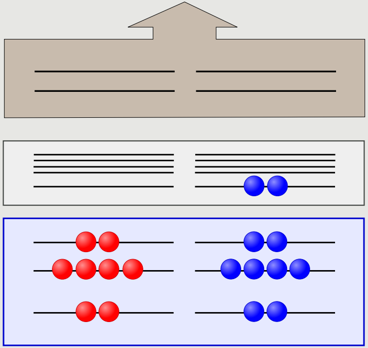


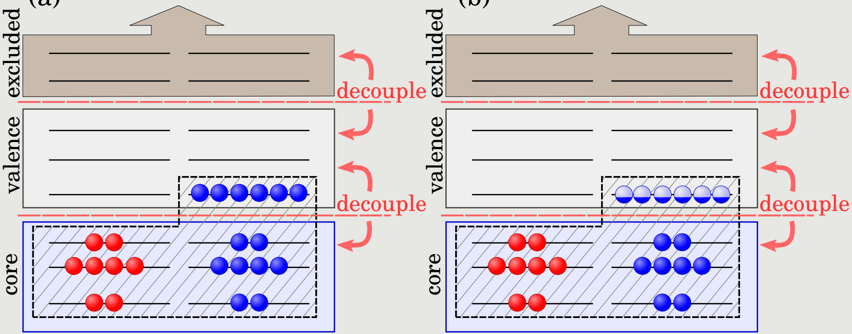
Tsukiyama et al. (2012), Hergert et al. (2013), Bogner et al. (2014)

What reference should be used when decoupling a valence space?

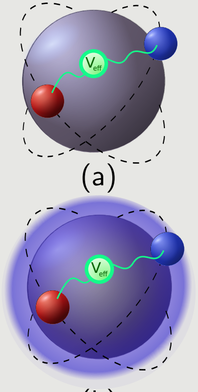
# Ensemble normal ordering

$$H = E_0 + \sum_{ij} f_{ij}\{a_i^\dagger a_j\} + \frac{1}{4}\sum_{ijkl}\Gamma_{ijkl}\{a_i^\dagger a_j^\dagger a_l a_k\} + \frac{1}{36}\sum_{ijklmn} W_{ijklmn}\{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}$$

$$\langle\Phi_0|\{a_i^\dagger \dots a_N\}|\Phi_0\rangle = 0 \qquad \mathrm{Tr}\left(\rho\{a_i^\dagger \dots a_N\}\right) = 0$$

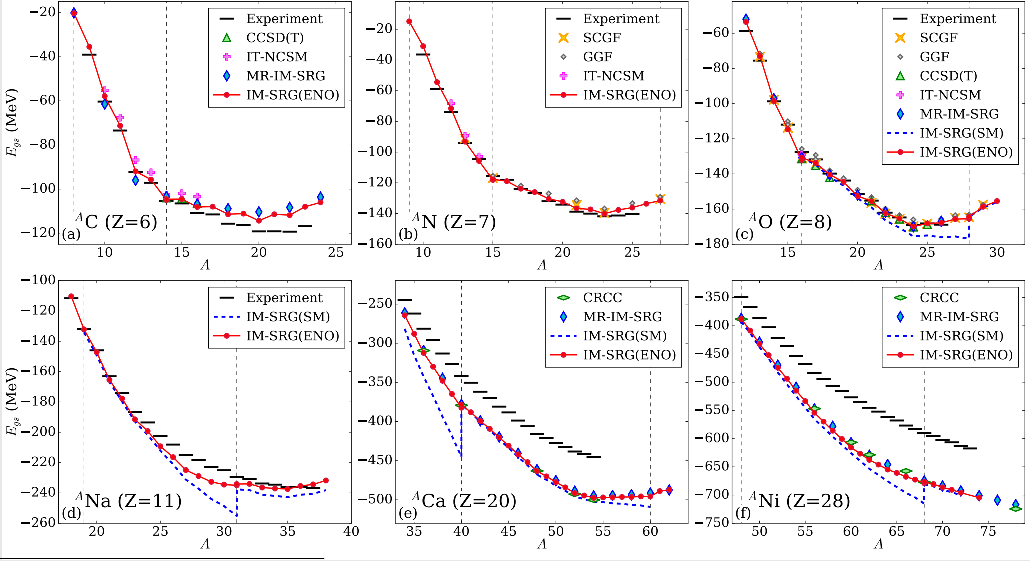



$$|\Phi_0\rangle = |^{22}\mathrm{O}\rangle \qquad \rho = \sum_\alpha c_\alpha |\Phi_\alpha\rangle\langle\Phi_\alpha|$$



(a)
(b)

# Ground state energies




SRS et al. PRL (2017)

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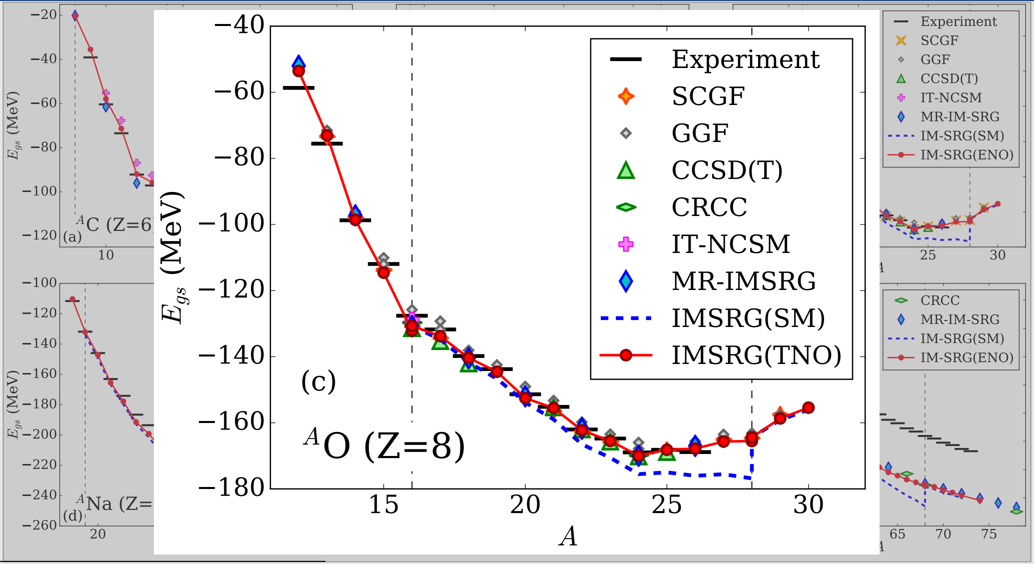


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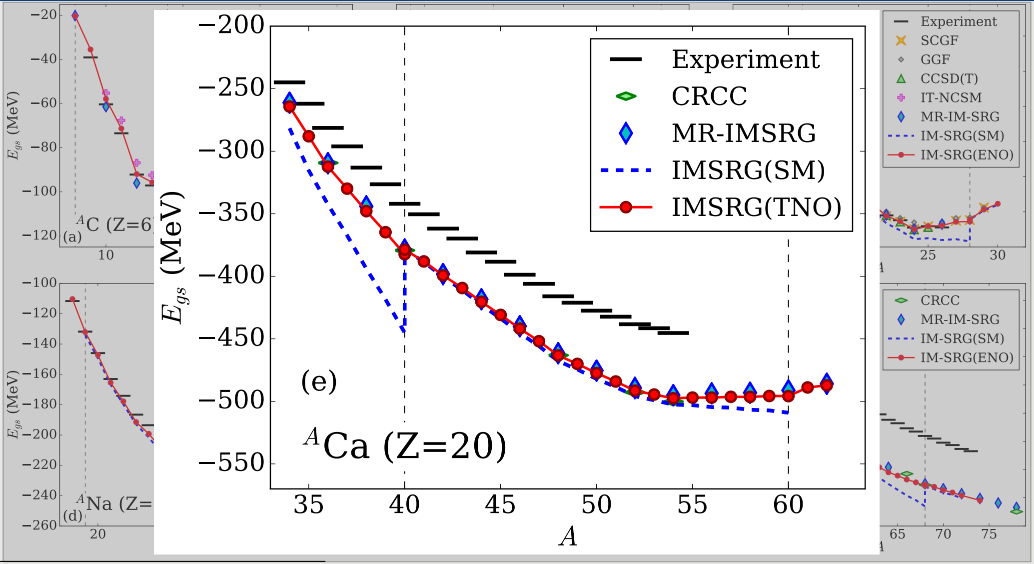
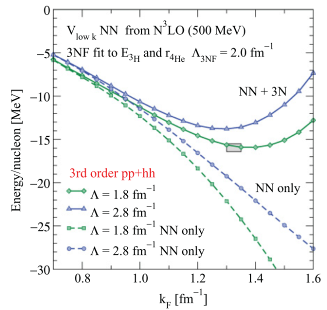



SRS et al. PRL (2017)

| | EM 500/400 | EM 1.8/2.0 |
|---|---|---|
| NN | $N^3LO$<br>$\Lambda_{2N} = 500$ MeV<br>non-local regulator<br>fit to $NN$ scattering, $^2$H<br>$\lambda_{SRG} = 1.88$ fm$^{-1}$ | same<br>same<br>same<br>same<br>$\approx$ same |
| 3N | $N^2LO$<br>$\Lambda_{3N} = 400$ MeV<br>**local regulator**<br>**fit to $^3$H BE, $t_{1/2}$**<br>**consistently SRG evolved** | same<br>$\approx$ same<br>**non-local regulator**<br>**fit to $^3$H BE, $^4$He $r_{ch}$**<br>**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. (in prep.)

# Saturation and finite nuclei

| | EM 500/400 | EM 1.8/2.0 |
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| | non-local regulator | same |
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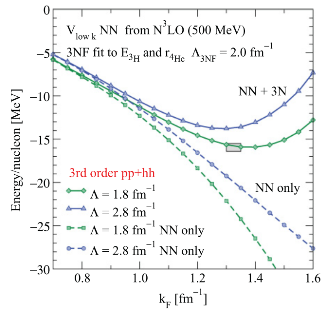
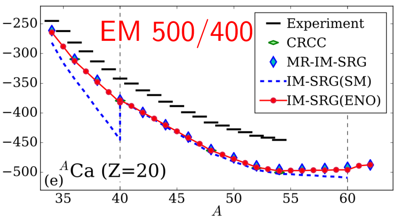
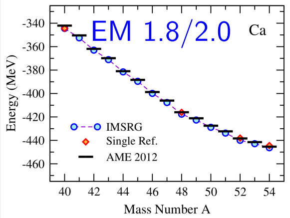
| | **consistently SRG evolved** | **no SRG for 3N** |

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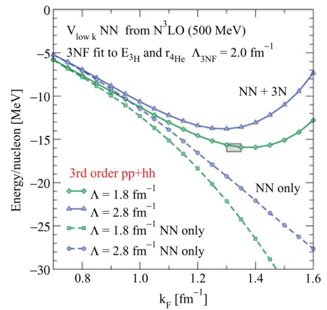
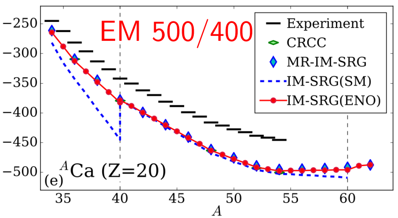
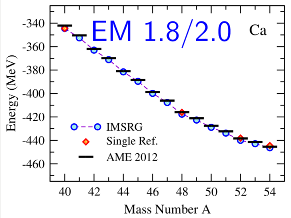
| | **consistently SRG evolved** | **no SRG for 3N** |



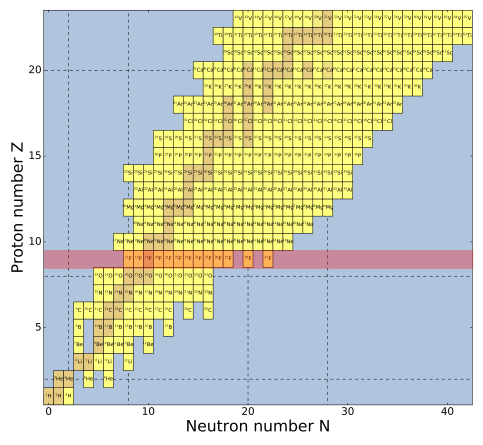

- Neither interaction is fully consistent

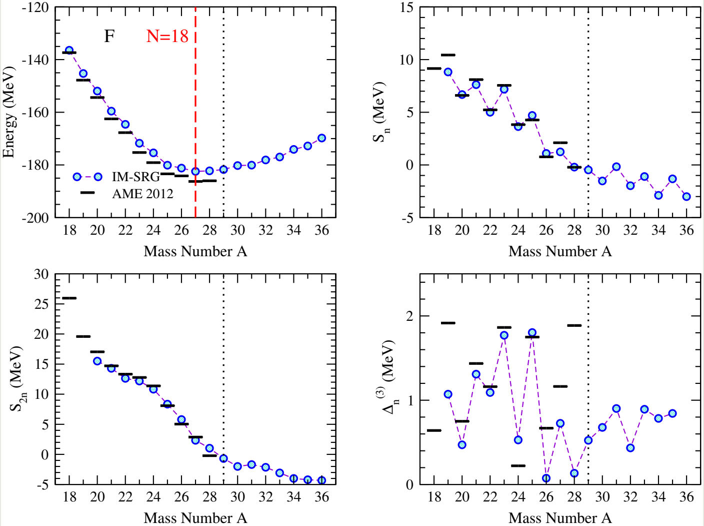
  however. . .

- 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. (in prep.)

# EM 1.8/2.0 interaction



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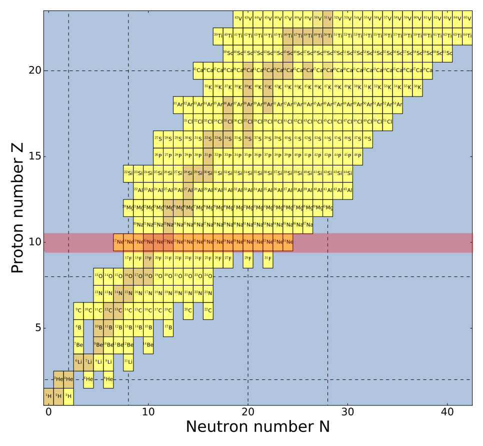


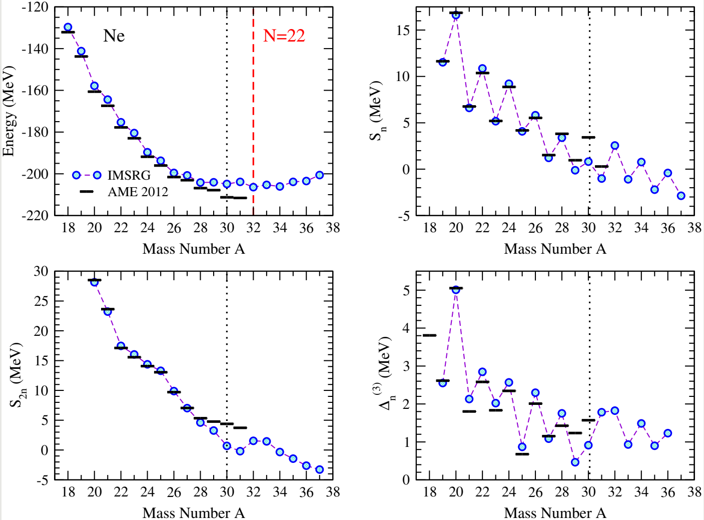

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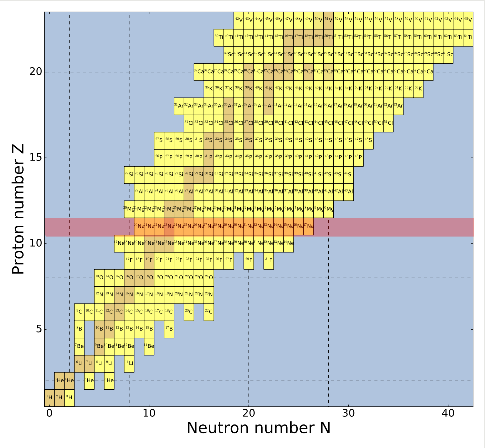


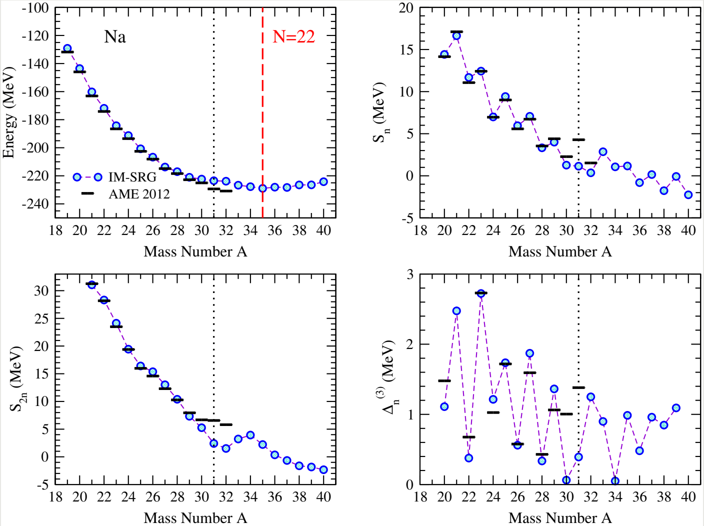

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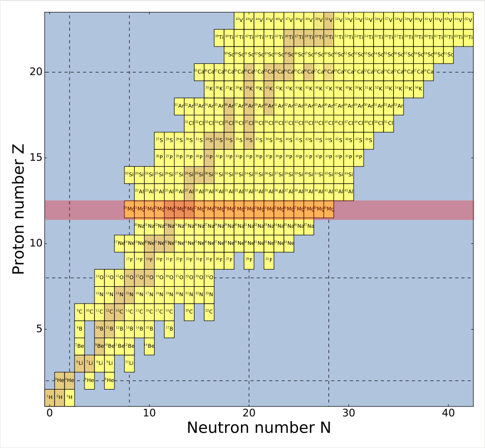


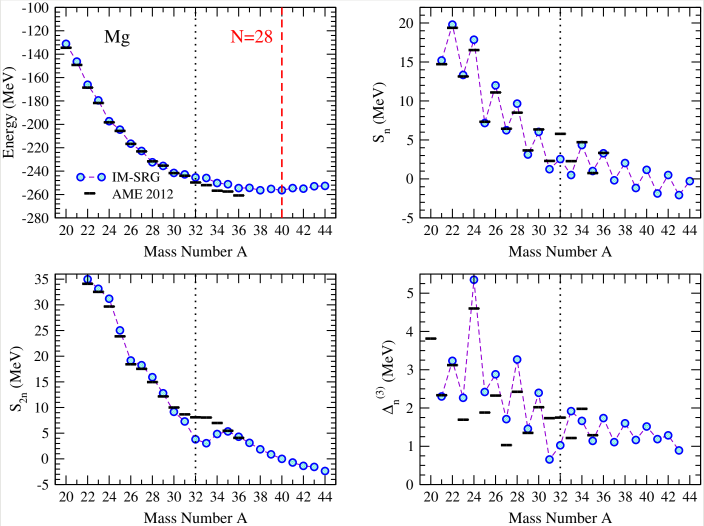

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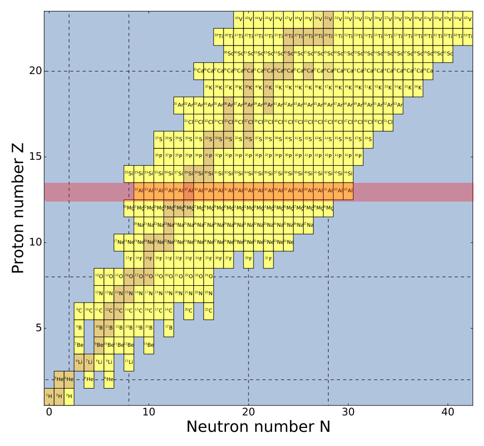


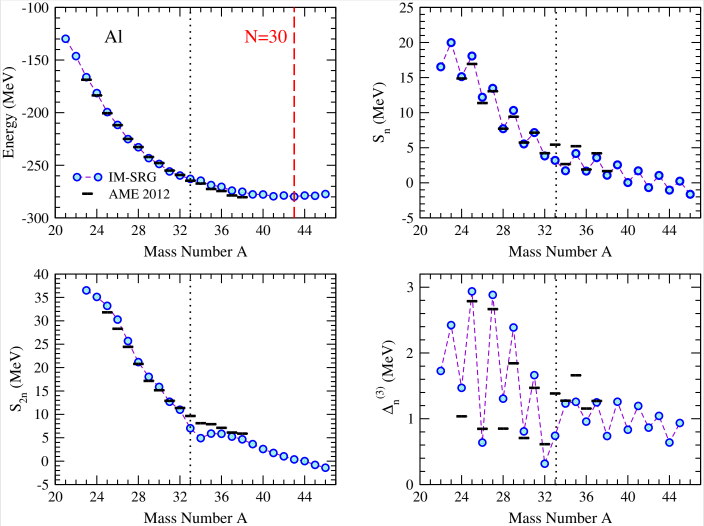

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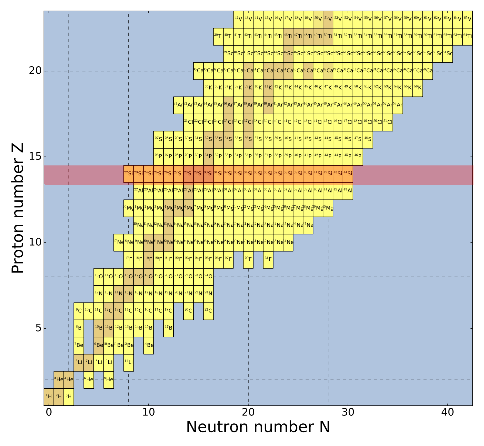


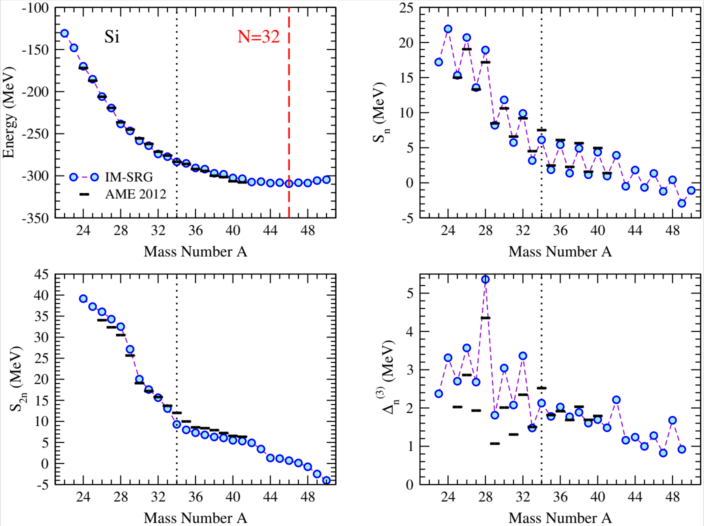

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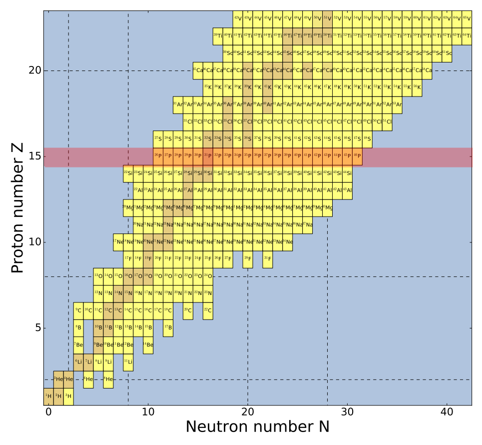


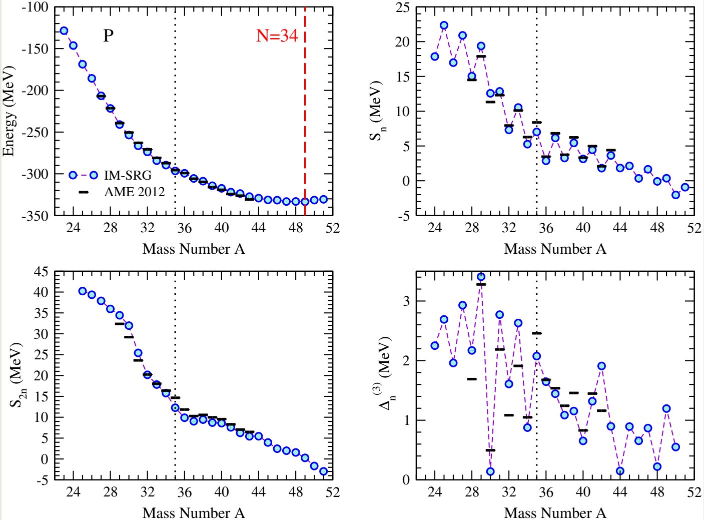

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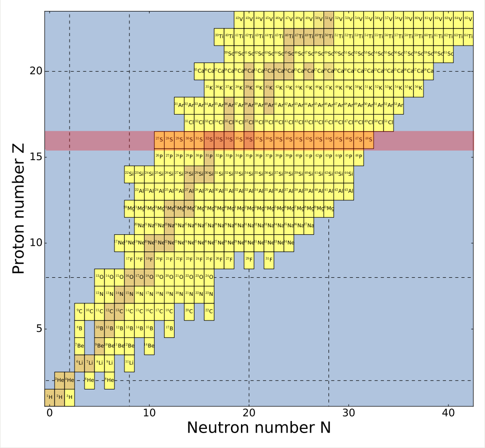


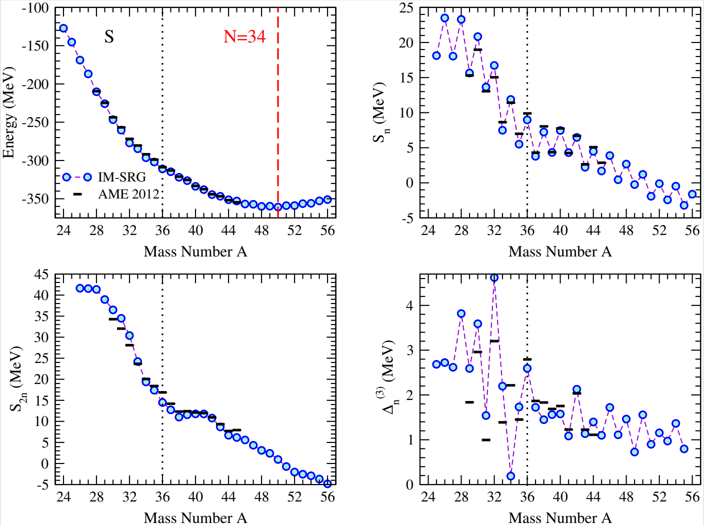

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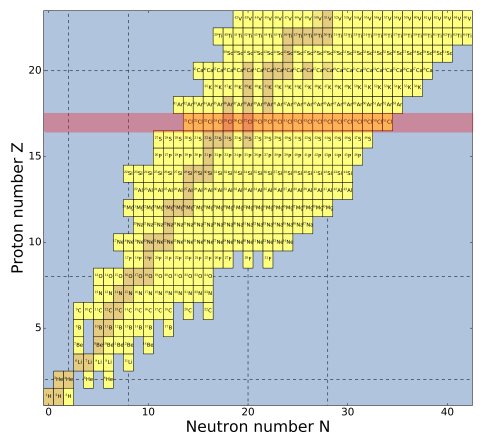
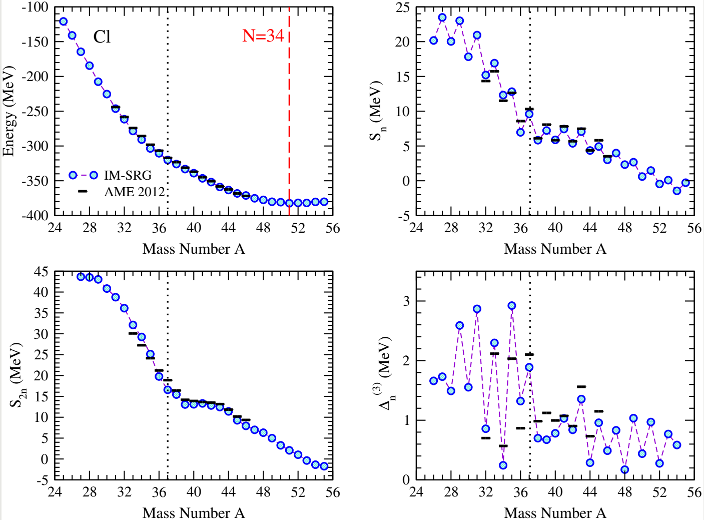
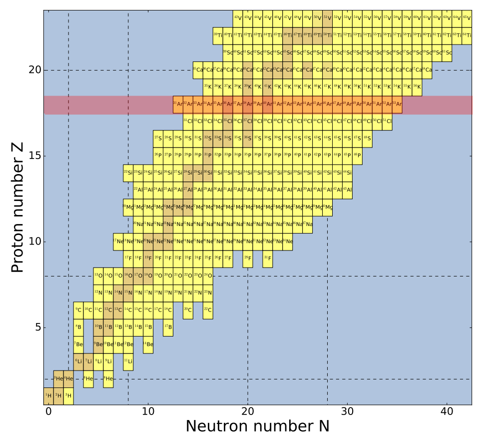
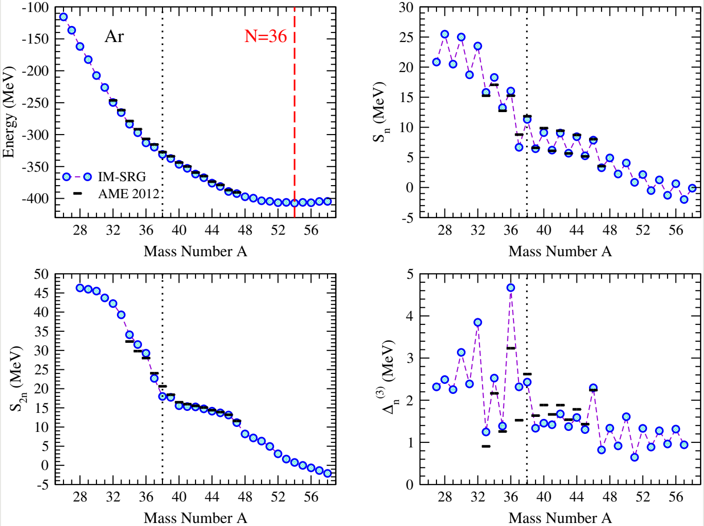


# EM 1.8/2.0 interaction



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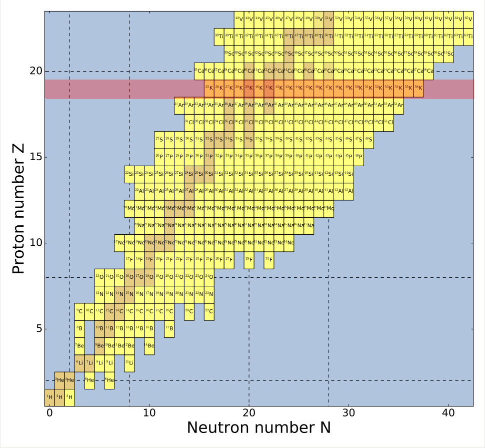
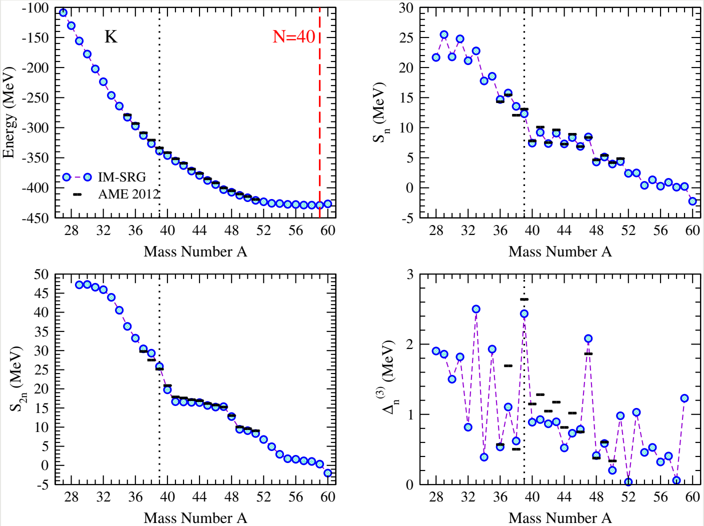
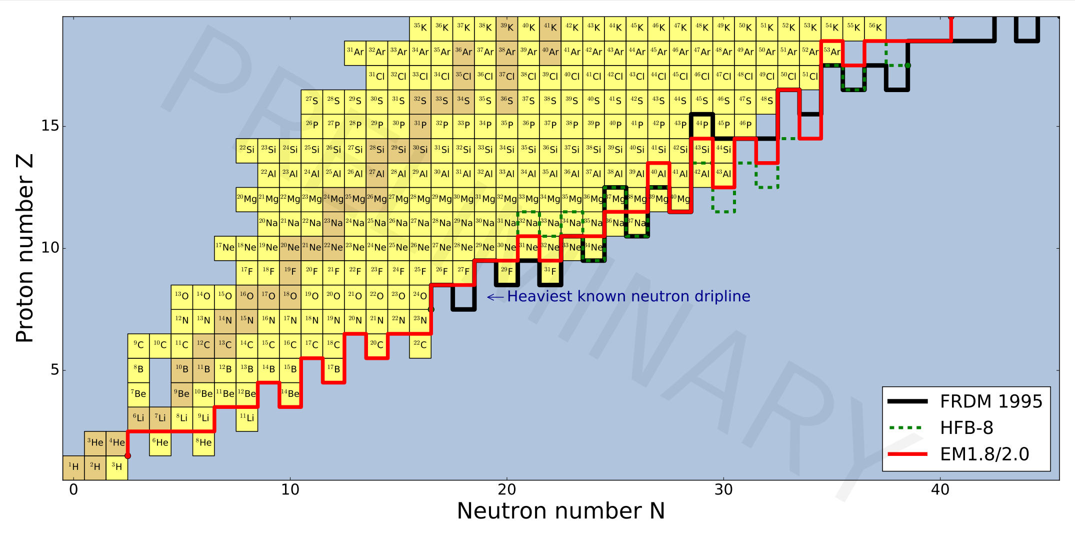
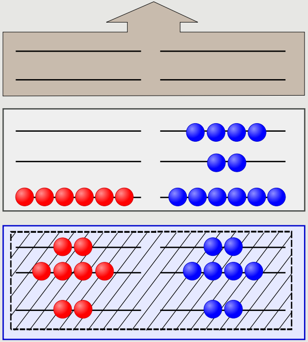


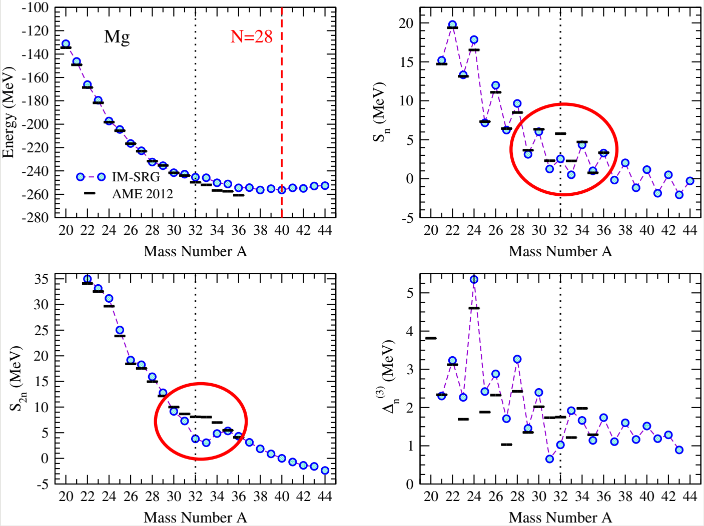






Baumann et al. Nature (2007), Möller et al. (1995), Samyn et al. (2004), Holt et al. (in prep.)

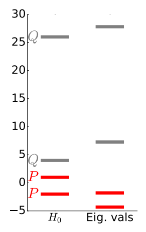
# Non-standard valence spaces

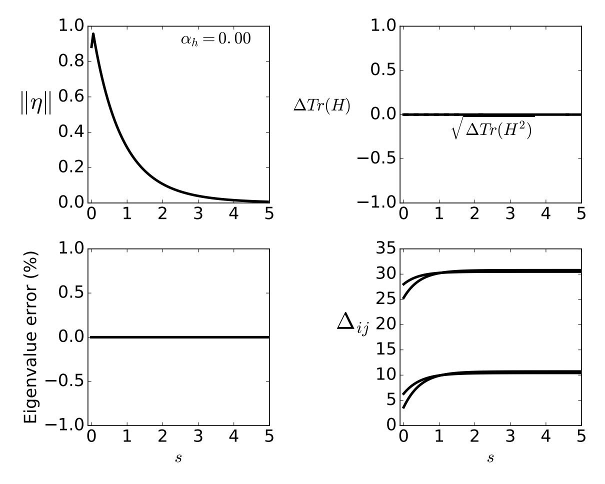




First, a toy problem:

$$H = \begin{pmatrix} 1 & 5 & 0 & 5 \\ 5 & 26 & 5 & 0 \\ 0 & 5 & -2 & 1 \\ 5 & 0 & 1 & 4 \end{pmatrix}$$




$$\eta = \frac{1}{2}\mathrm{atan}\left(\frac{2H_{qp}}{H_{qq}-H_{pp}}\right) - h.c.$$

$$H(s+\delta s) = e^{\eta_s \delta s} H(s) e^{\eta_s^\dagger \delta s}$$

Suzuki, Prog. Theor. Phys. (1977), L. Kemmler student project

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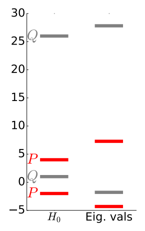


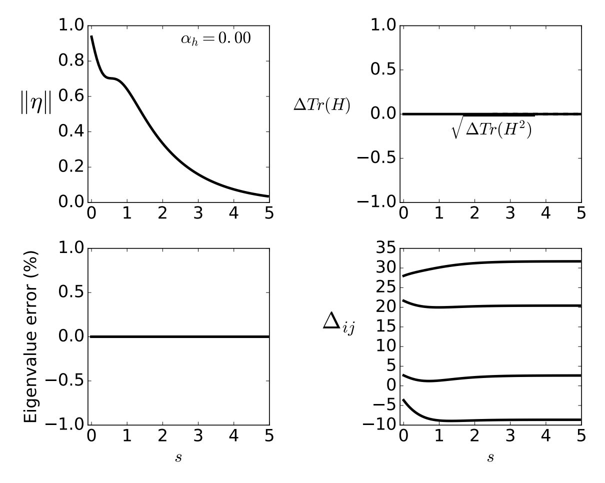


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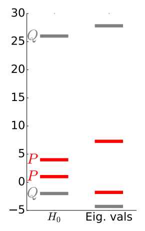


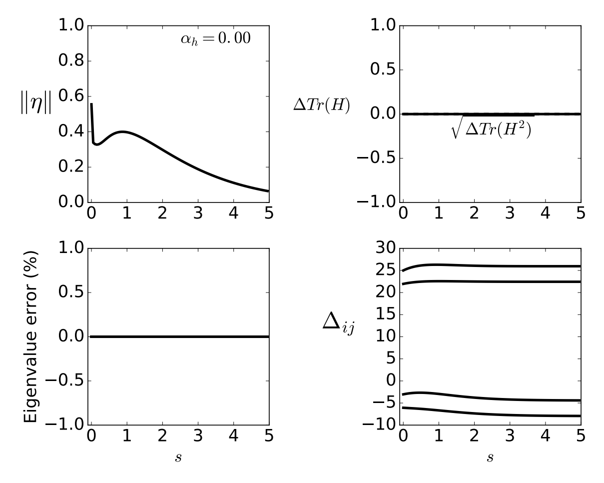


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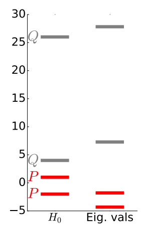


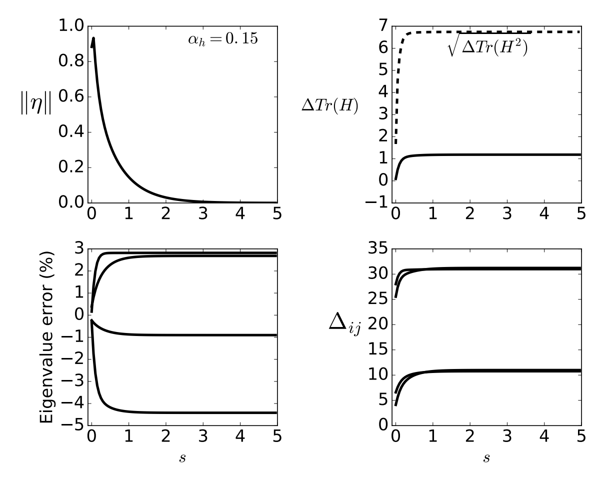


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break unitarity: $\eta \rightarrow \eta + \alpha_h[\eta, H]$

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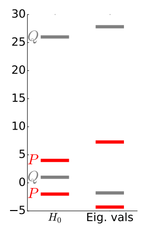


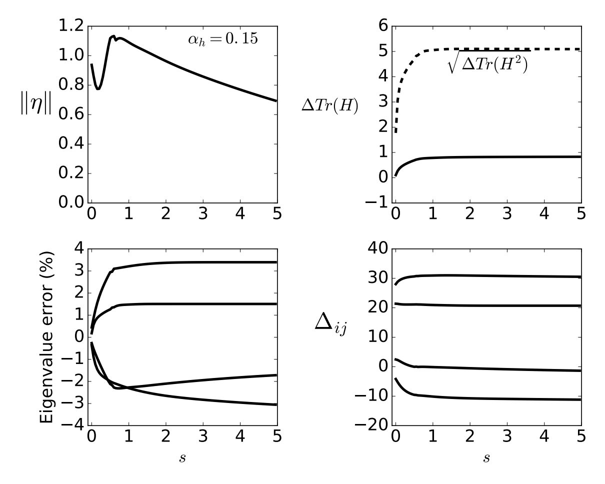


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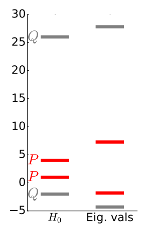


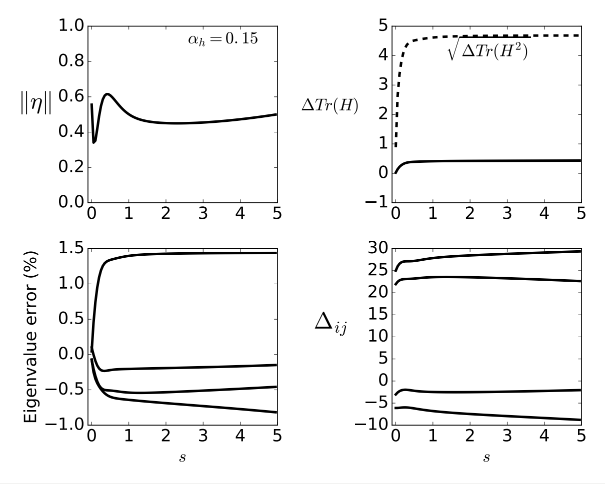


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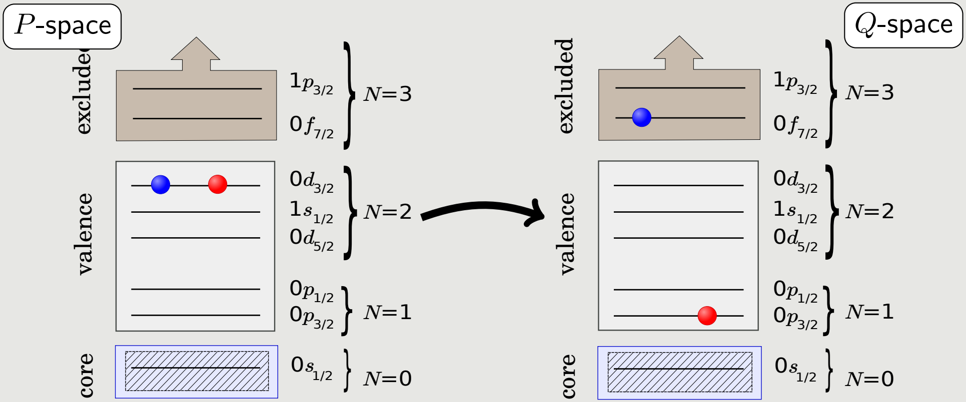
Suzuki, Prog. Theor. Phys. (1977), L. Kemmler student project

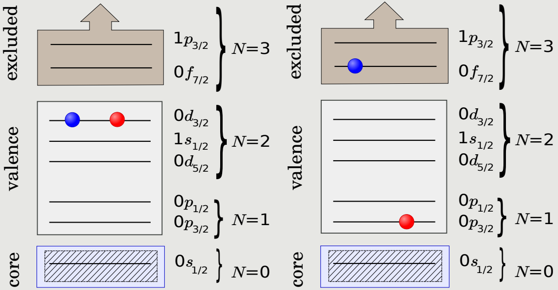


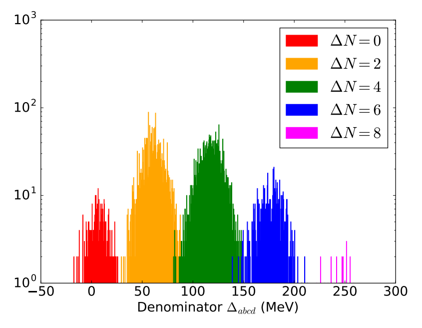

$$\eta_s = \frac{1}{2}\mathrm{atan}\left(\frac{2H_{qp}(s)}{H_{qq}(s)-H_{pp}(s)}\right) - h.c.$$

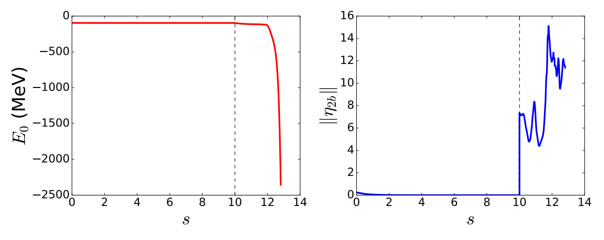
$\Delta N = 0 \rightarrow$ **negative denominators**

# Non-standard valence spaces

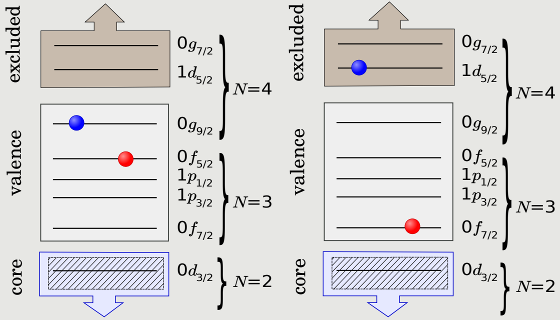
## $psd$ space, $^{16}$O reference

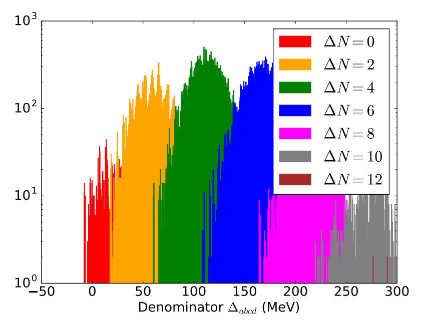


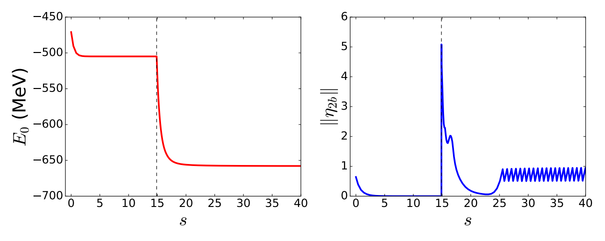



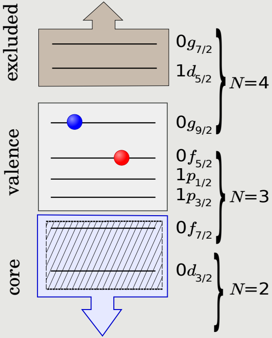
$pfg_9$ space, $^{76}$Ge reference

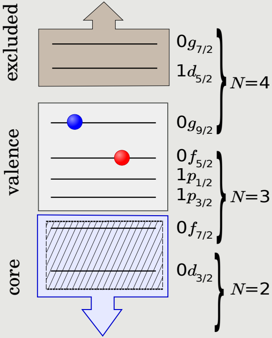


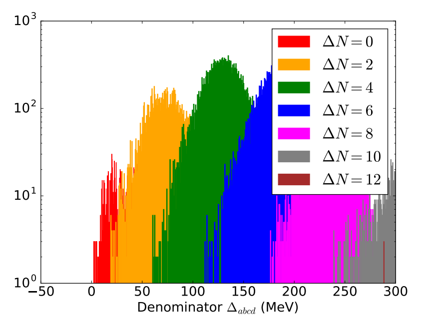



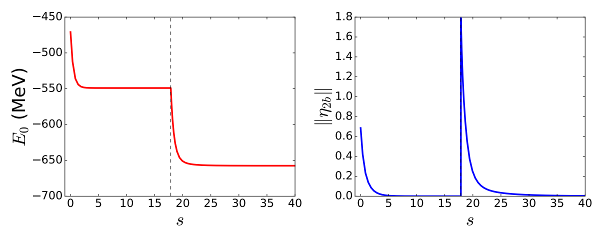



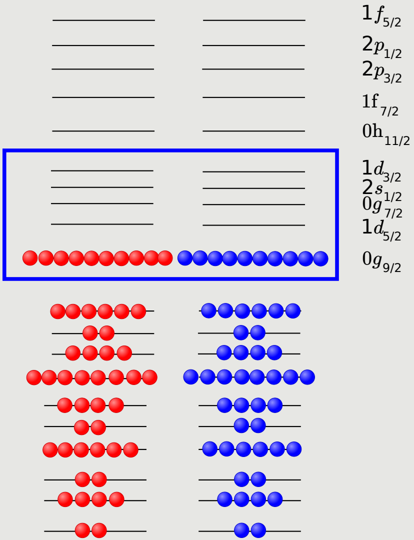
# $pf_5g_9$ space, $^{76}$Ge reference

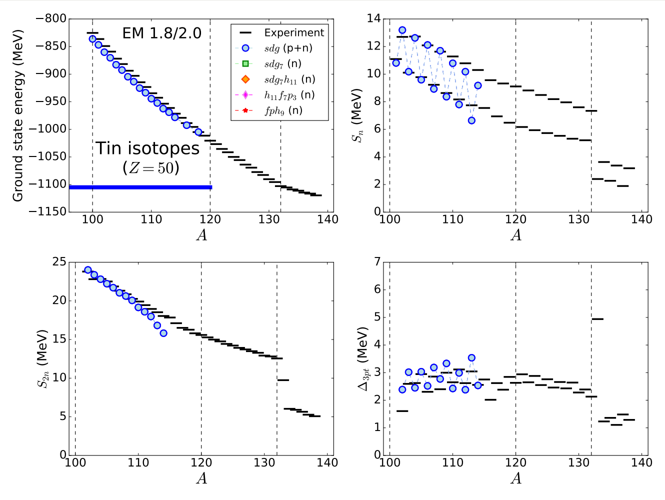


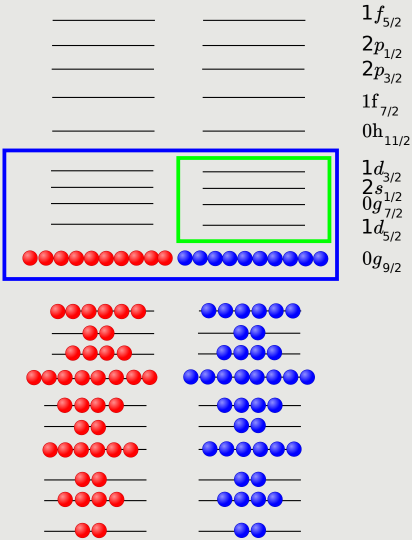



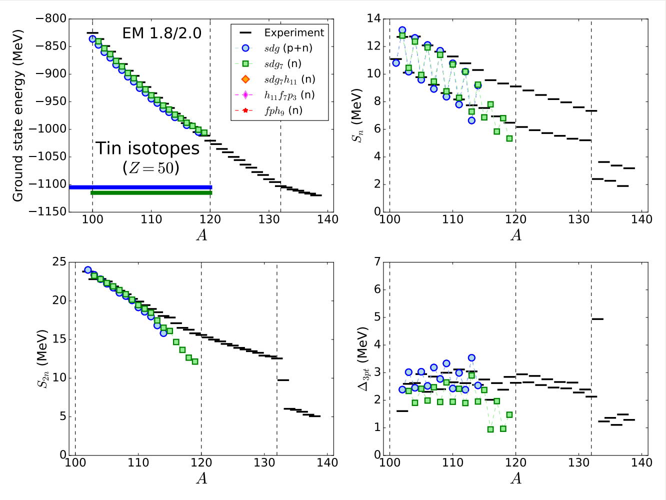




$1f_{5/2}$
$2p_{1/2}$
$2p_{3/2}$
1f$_{7/2}$
0h$_{11/2}$
$1d_{3/2}$
$2s_{1/2}$
$0g_{7/2}$
$1d_{5/2}$
$0g_{9/2}$


EM 1.8/2.0
Tin isotopes
$(Z=50)$
Ground state energy (MeV)
Experiment
$sdg$ (p+n)
$sdg_7$ (n)
$sdg_7h_{11}$ (n)
$h_{11}f_7p_3$ (n)
$fph_9$ (n)
$S_n$ (MeV)
$S_{2n}$ (MeV)
$\Delta_{3pt}$ (MeV)
$A$

# Non-standard valence spaces



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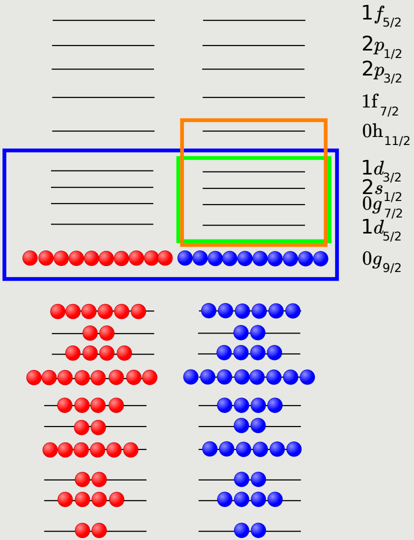


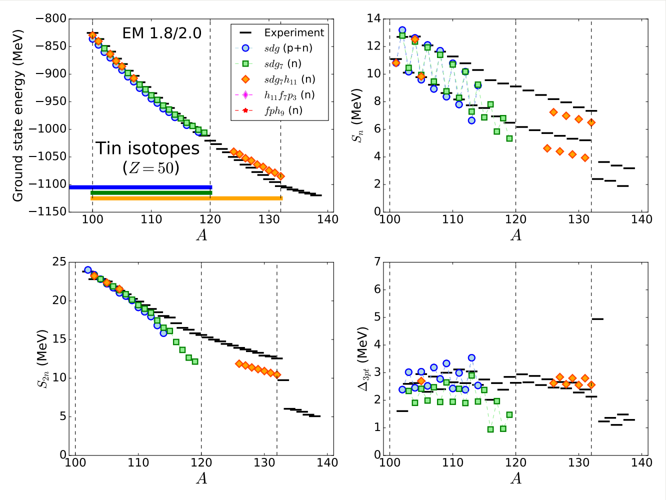

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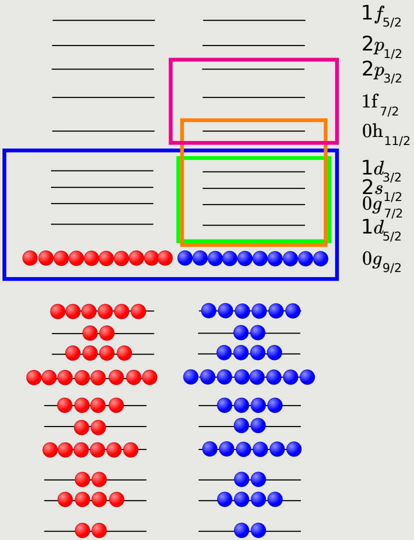


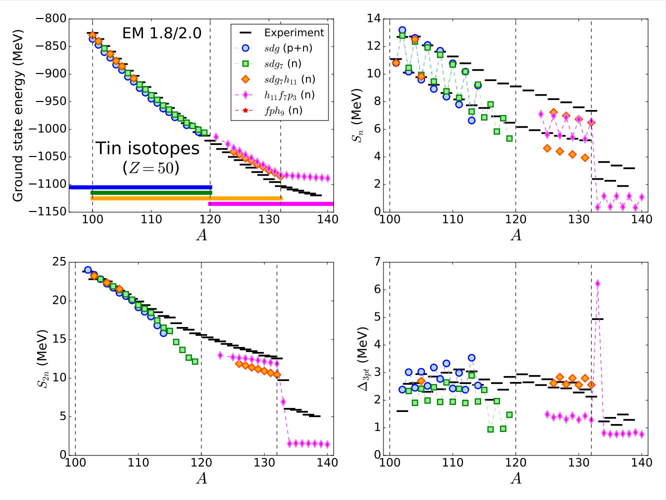

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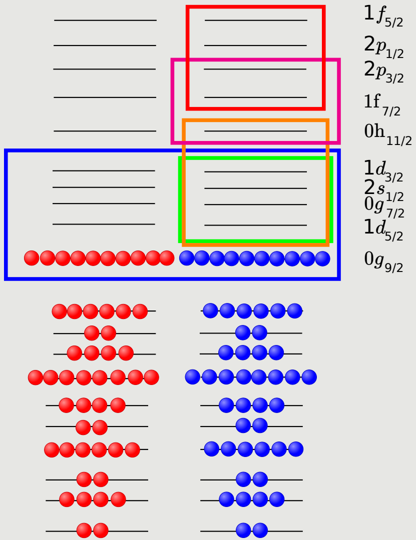


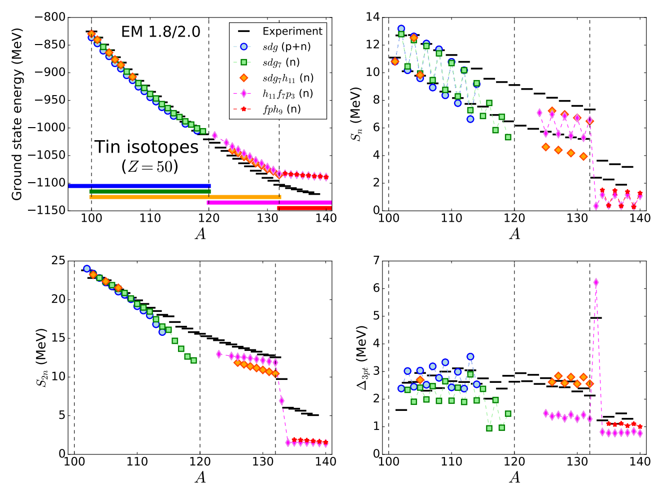

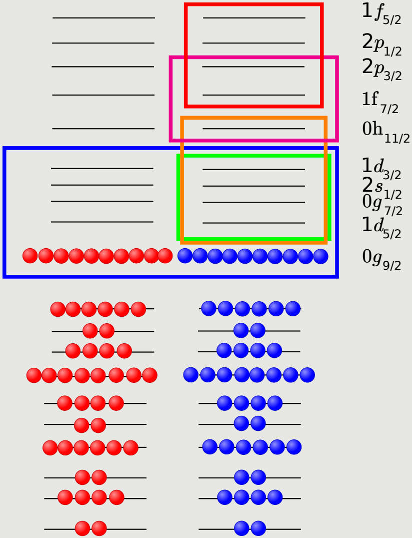
$1f_{5/2}$
$2p_{1/2}$
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1f$_{7/2}$
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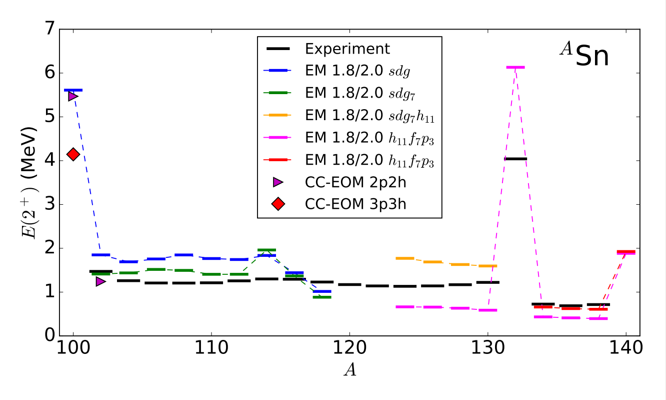
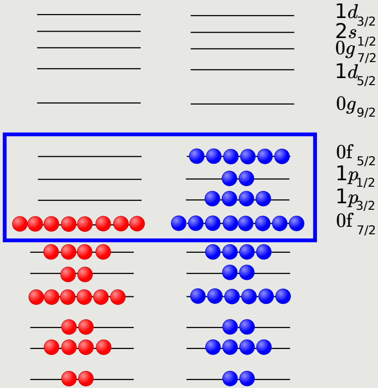
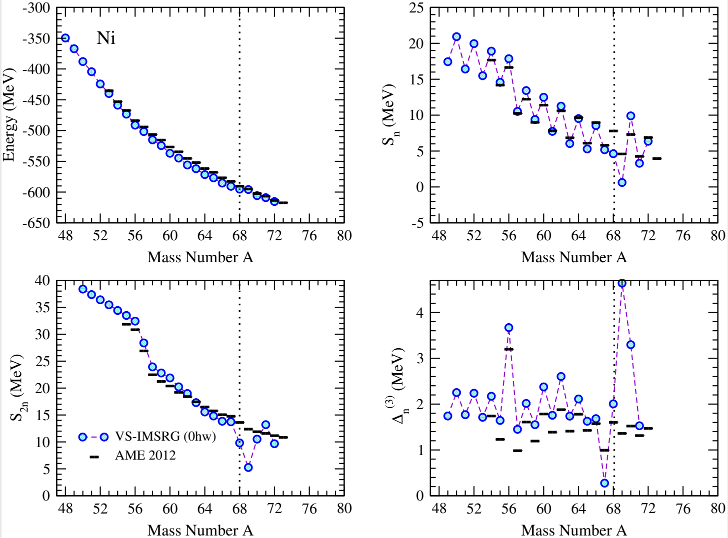
$1d_{3/2}$
$2s_{1/2}$
$0g_{7/2}$
$1d_{5/2}$
$0g_{9/2}$


$^{A}$Sn
Experiment
EM 1.8/2.0 $sdg$
EM 1.8/2.0 $sdg_7$
EM 1.8/2.0 $sdg_7h_{11}$
EM 1.8/2.0 $h_{11}f_7p_3$
EM 1.8/2.0 $h_{11}f_7p_3$
CC-EOM 2p2h
CC-EOM 3p3h
$E(2^+)$ (MeV)
$A$
0
1
2
3
4
5
6
7
100
110
120
130
140

# Non-standard valence spaces



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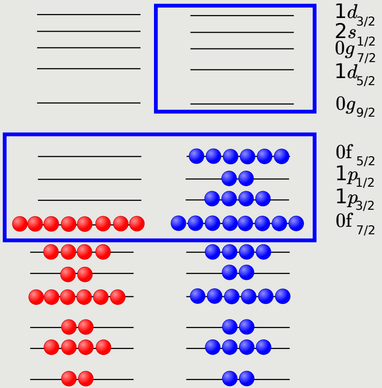


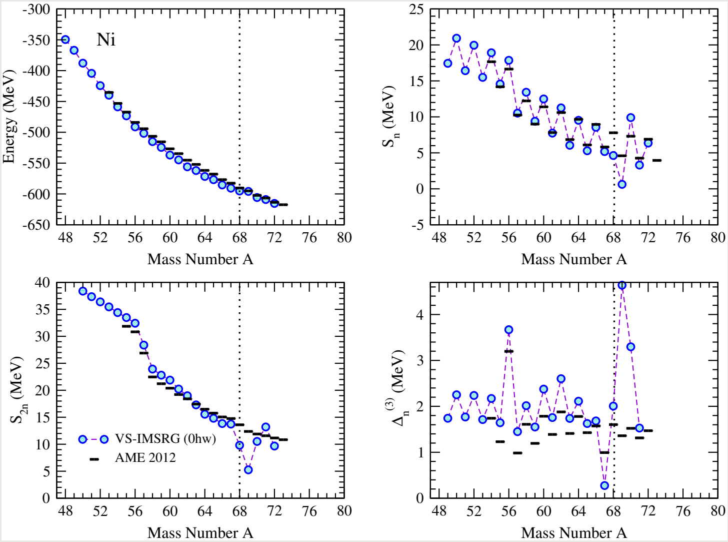

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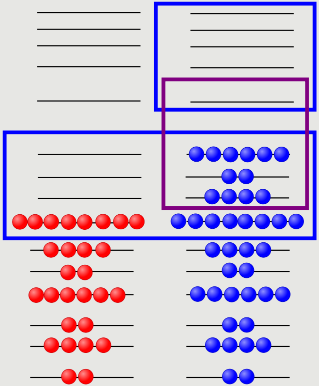
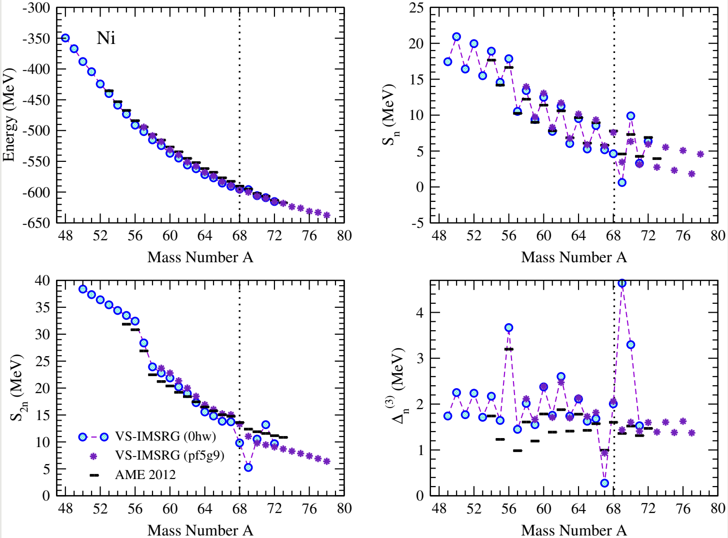
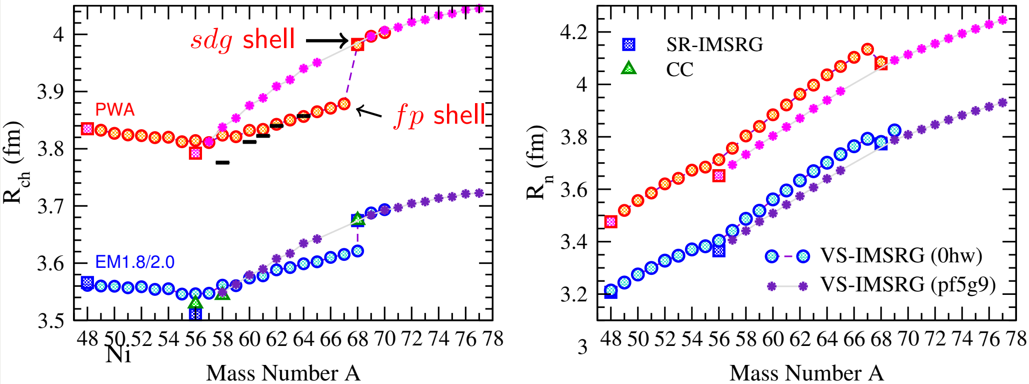


# Radii of nickel isotopes



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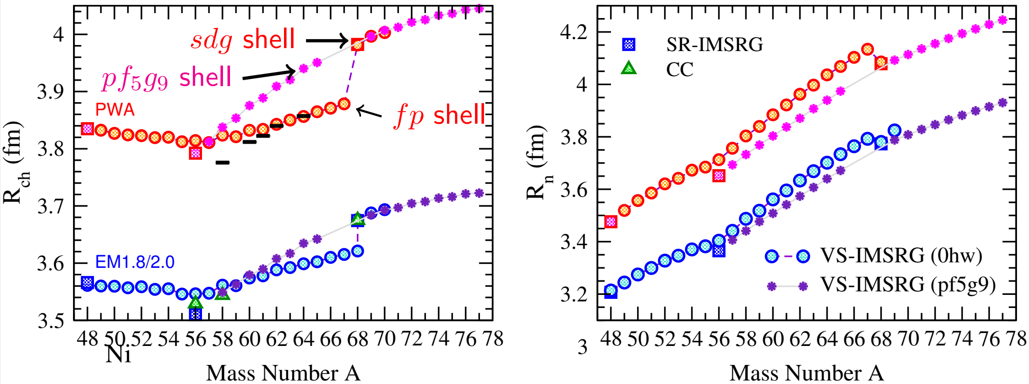
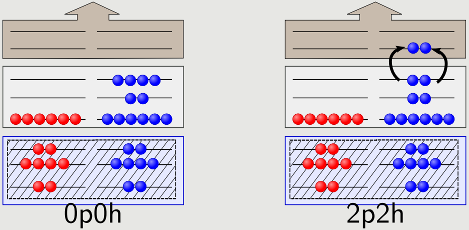
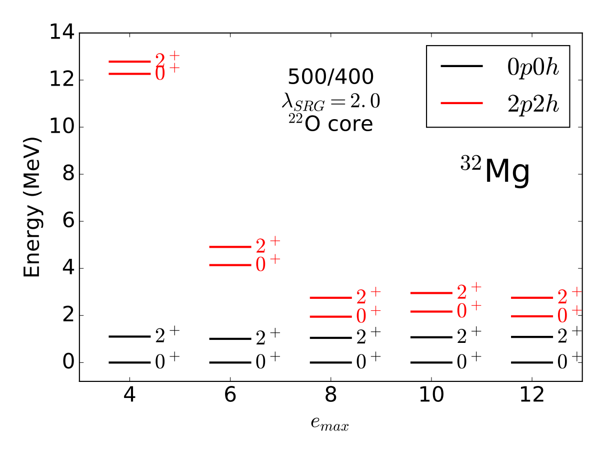





$^{22}$O core

$sd_3 f_7 p_3$ valence space for neutrons

$sd$ valence space for protons



## Approximations:

- $e_{max}$, $E_{3max}$
- NO2B, IM-SRG(2)

## "Arbitrary choices":

- $\hbar\omega$ for oscillator basis
- Generator $\eta$
- Reference $|\Phi_0\rangle$ (or $\rho$)
- Valence space

- The "choices" should be made to minimize the amount left out by the approximations.
- Eliminate approximations $\rightarrow$ result independent of choices.
- Dependence on choices $\rightarrow$ estimate of approximation error
- Other ways to estimate error:
  - Extrapolations
  - Perturbative estimate of e.g. 3-body terms
  - Invariant trace?

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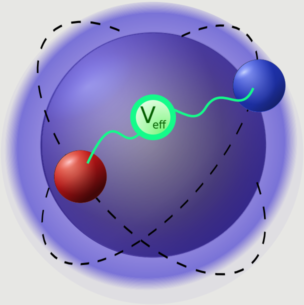
# Summary




- Valence space IM-SRG with ensemble normal ordering allows access to all nuclei up to A$\sim 100$
- Cost and accuracy comparable to closed-shell IM-SRG
- Consistent operators for transitions (see poster by N. Parzuchowski)
- Development of non-standard valence spaces extends this reach and improves results at the edge of the valence space
- Limit in $A$ is due to $E_{3max}$ truncation
- Calculations with multiple valence spaces probes truncation error

Collaborators:

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

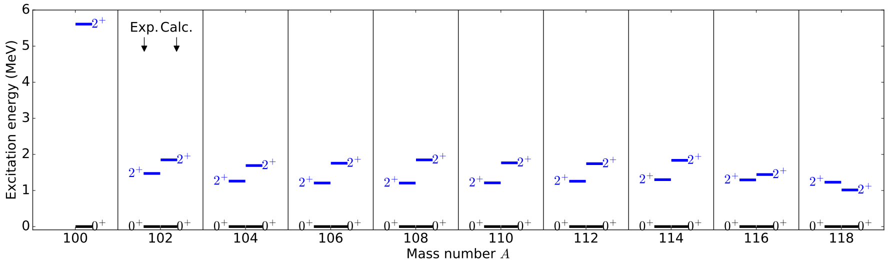
NSCL/MSU S. Bogner, H. Hergert, N. Parzuchowski

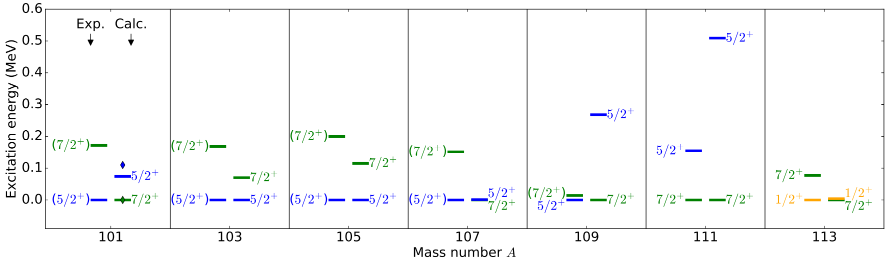
TU Darmstadt R. Roth, A. Schwenk, J. Simonis, C. Stumpf

ORNL/UT G. Hagen, T. Morris

# Backup slides

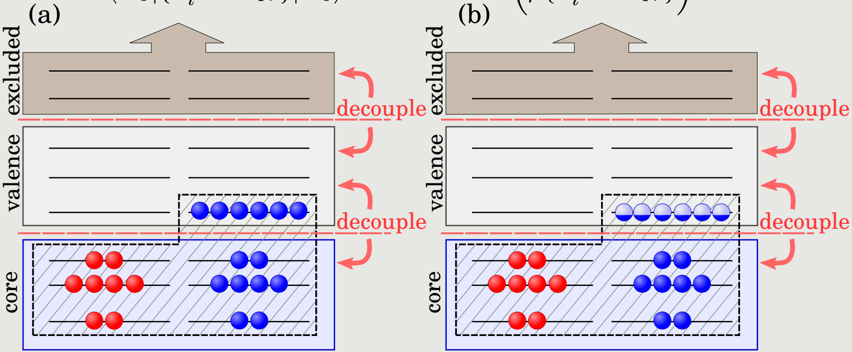
# Spectroscopy of tin isotopes



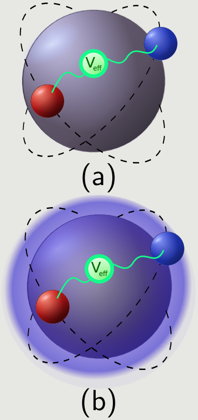



$$H = E_0 + \sum_{ij} f_{ij}\{a_i^\dagger a_j\} + \frac{1}{4}\sum_{ijkl}\Gamma_{ijkl}\{a_i^\dagger a_j^\dagger a_l a_k\} + \frac{1}{36}\sum_{ijklmn} W_{ijklmn}\{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}$$

$$\langle\Phi_0|\{a_i^\dagger \dots a_N\}|\Phi_0\rangle = 0 \qquad \text{Tr}\left(\rho\{a_i^\dagger \dots a_N\}\right) = 0$$

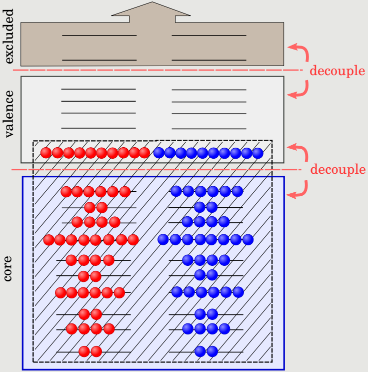


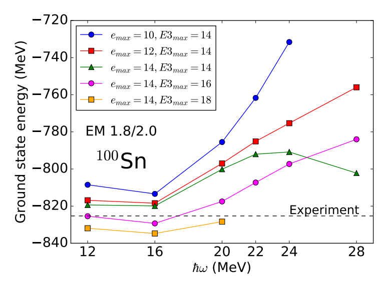

$$|\Phi_0\rangle = |^{22}\text{O}\rangle \qquad \rho = \sum_\alpha c_\alpha |\Phi_\alpha\rangle\langle\Phi_\alpha|$$



# The tin isotopes ($Z = 50$)

- $^{100}$Sn: 50 protons, 50 neutrons
- Open shell valence space: full $gds$ shell
- $m$-scheme dimension $\sim 10^{12}$
- Need importance truncation to diagonalize!

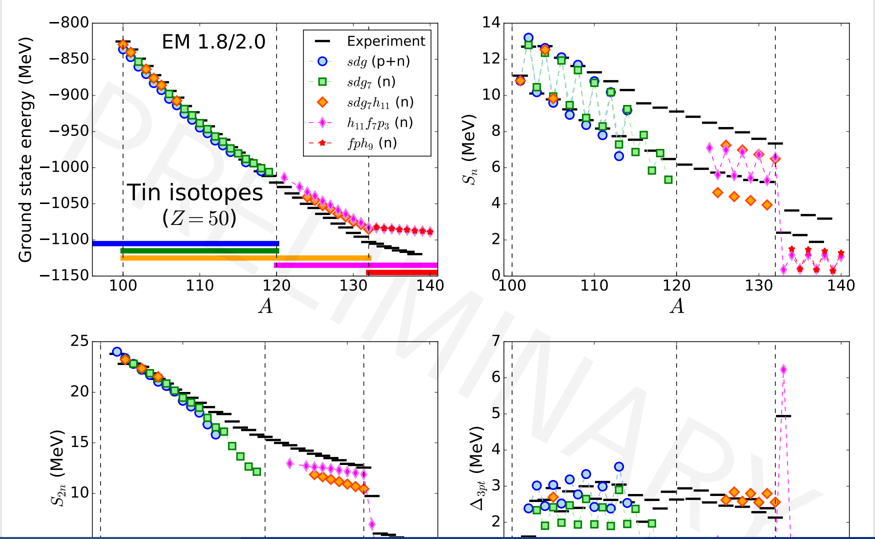


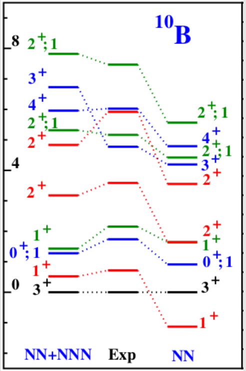

| $E_{3max}$ | Storage (GB) |
|---|---|
| 14 | 5 |
| 16 | 20 |
| 18 | 100 |

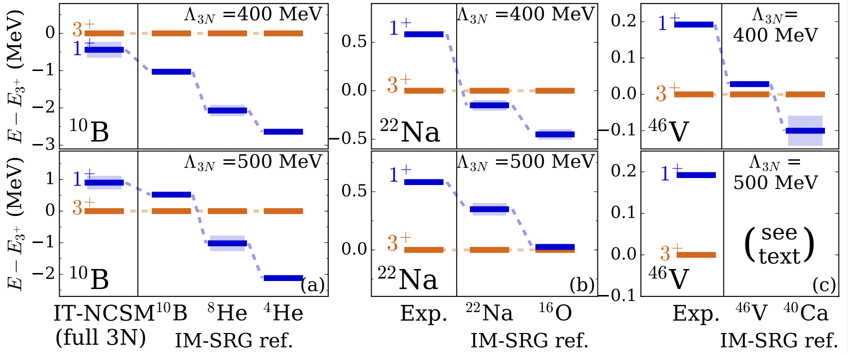
Simonis et al. (in prep.), Stumpf et al. PRC(R) (2016)

Isotopic chain with $\hbar\omega = 16$, $e_{max} = 14$, $E3_{max} = 16$

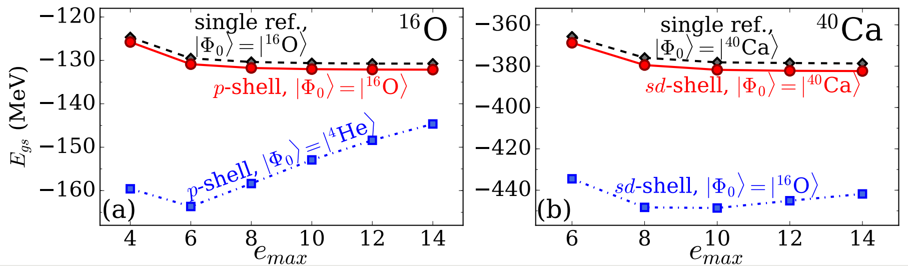


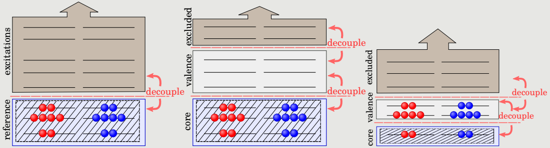
# Capturing valence 3N effects w/ NN machinery:




Navrátil et al. PRL (2007), SRS et al. PRL (2017)



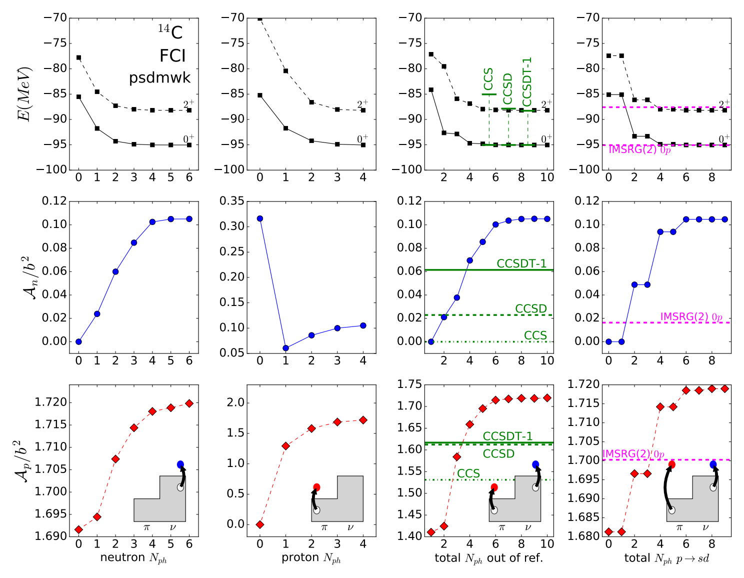




- Convergence not possible without proper normal ordering reference
- Two competing effects
  - Missing 3N forces
  - Bad single particle basis
- ∼1% error due to additional decoupling

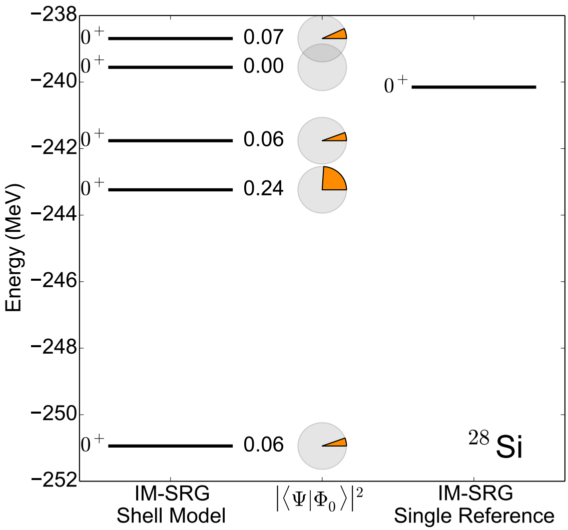
# How well does it work?

## What's going on?

- Toy problem: $^{14}$C, $p$-$sd$ space
- $\mathcal{A}_p \equiv |\langle 0^+ \| r_p^2 Y_p^{(2)} \| 2^+ \rangle|$
- Truncate FCI in $N$p-$N$h excitations
- Compare FCI with coupled cluster (from Gaute Hagen) and IM-SRG
  - CCSDT-1: singles+doubles+≈triples
- Missing p-h excitations: unimportant for energy, important for $E2$



# Picking out spherical excited states



What *can't* we do, and why isn't everything perfect?

- **So far, limited to valence spaces defined by a single major oscillator shell**
  - No intruder states
  - No "island of inversion" states
  - No excited states of $^{4}$He, $^{16}$O, $^{28}$O, $^{40}$Ca, $^{60}$Ca, $^{80}$Zr ($\leftarrow$ EOM can do these)
  - Max. 70 protons, 70 neutrons (oscillator magic numbers: 2, 8, 20, 40, 70, 112. . . )
- Large space limited to $\sim$15 major oscillator shells (usually sufficient)
- **Limited to IM-SRG(2) approximation**
- Continuum states not included
- **Current input chiral interactions are not perfect**

## Technical aside:

Recall the transformed Hamiltonian:

$$\tilde{H} = UHU^\dagger$$

Other operators may be transformed consistently.
If the operator $\mathcal{O}^\lambda$ carries angular momentum $\lambda$, then

$$\tilde{\mathcal{O}}^\lambda = U\mathcal{O}^\lambda U^\dagger$$

$$e^{\Omega}\mathcal{O}^\lambda e^{-\Omega} = \mathcal{O}^\lambda + [\Omega, \mathcal{O}^\lambda] + \frac{1}{2}[\Omega, [\Omega, \mathcal{O}^\lambda]] + \dots$$

Only additional work is to derive angular momentum coupled commutator expressions (done).

## Work in progress:

- Understand (and remedy) lack of $E2$ strength
- Understand quenching of Gamow-Teller strength
- Neutrinoless double beta decay (C. Payne†)
- Dark matter scattering (S. Leutheusser*)
- Improve IM-SRG(2) approximation
- Applications to atomic systems (D. Livermore*)

## Potential projects:

- Can medium-mass nuclei provide a filter for chiral interactions?
- Unify reaction and structure – ab initio optical potentials, electron scattering
- Connections to DFT
  - Can ab initio calculations provide additional “data” for fitting?
- Can we explicitly calculate collective model parameters?

†M.Sc. student, *Undergraduate