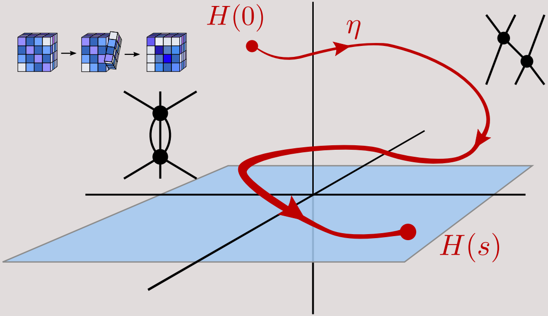
IMSRG with flowing 3N operators

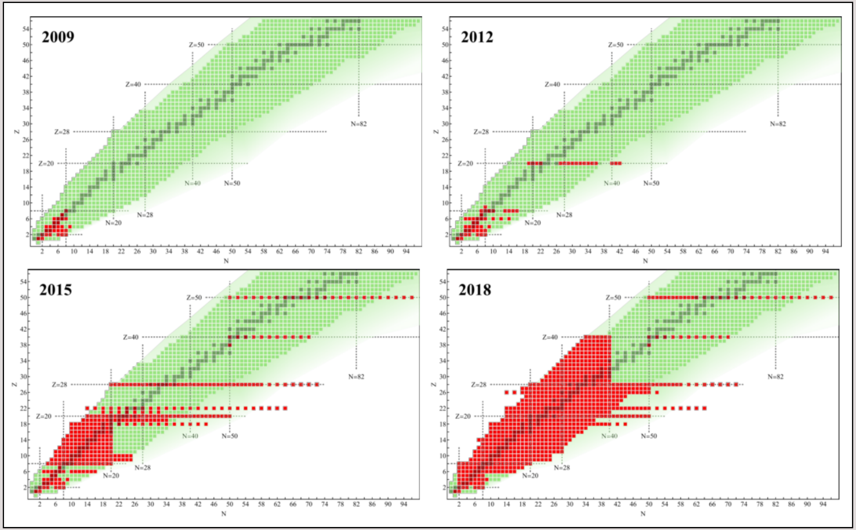
some first explorations



Ragnar Stroberg

University of Washington

Progress in Ab initio Techniques for Nuclear Physics
TRIUMF Vancouver, BC
March 5, 2020



Hebeler 2020; figure credit Heiko Hergert

$$H(s) = U(s) H U^{\dagger}(s)$$

$$\frac{dU}{ds} = \eta(s) U(s)$$

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

$$H(s) = H^{d}(s) + H^{od}(s)$$

$$H^{od}(s) \rightarrow 0 \text{ as } s \rightarrow \infty$$

Flow equations:

$$H(s) = U(s) H U^\dagger(s)$$

$$\frac{dU}{ds} = \eta(s) U(s)$$

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

$$H(s) = H^d(s) + H^{od}(s)$$

$$H^{od}(s) \to 0 \text{ as } s \to \infty$$

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

Flow equations:

$$\frac{dE_0}{ds} = [\eta(s), H(s)]_{0b}$$

$$\frac{df}{ds} = [\eta(s), H(s)]_{1b}$$

$$\frac{d\Gamma}{ds} = [\eta(s), H(s)]_{2b}$$

$$\frac{dW}{ds} = [\eta(s), H(s)]_{3b}$$

$$H(s) = U(s) H U^\dagger(s)$$

$$\frac{dU}{ds} = \eta(s) U(s)$$

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

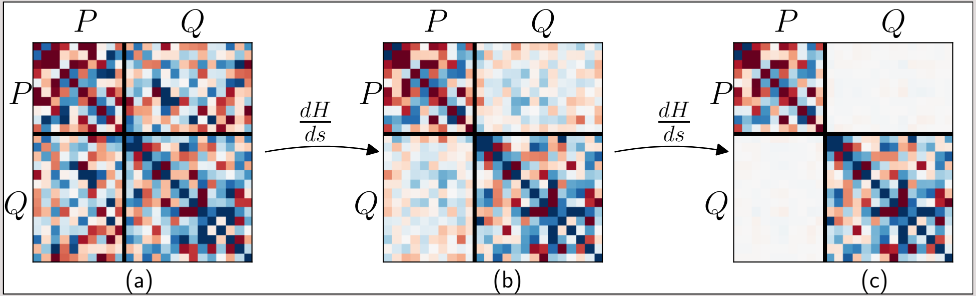
$$H(s) = H^d(s) + H^{od}(s)$$

$$H^{od}(s) \to 0 \text{ as } s \to \infty$$

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

Flow equations:
$$\frac{dE_0}{ds} = [\eta(s), H(s)]_{0b}$$
$$\frac{df}{ds} = [\eta(s), H(s)]_{1b}$$
$$\frac{d\Gamma}{ds} = [\eta(s), H(s)]_{2b}$$
$$\cancel{\frac{dW}{ds} = [\eta(s), H(s)]_{3b}}$$

$\boxed{\text{IMSRG(2)}}$



As $s \to \infty$, P space is decoupled from Q space.

Output is a shell model effective interaction
$\rightarrow$ diagonalize with NuShellX, Antoine, Kshell etc.

Stroberg et al. 2019

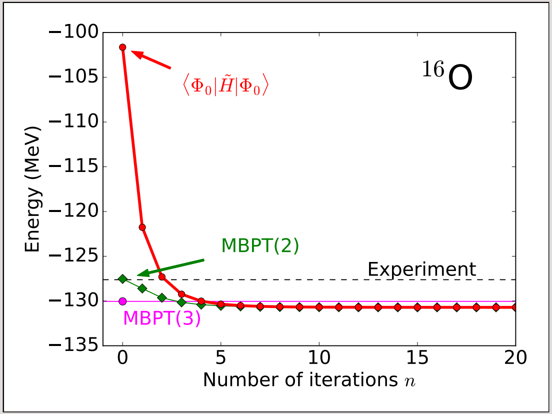
Magnus formulation of IMSRG

$$U(s) = e^{\Omega(s)} \quad \text{, Magnus operator } \Omega$$

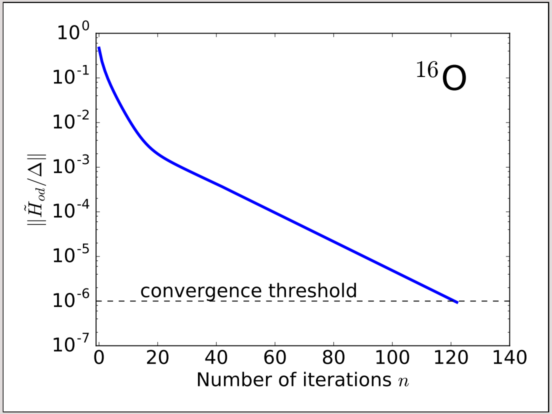
$$\begin{aligned} H(s) &= e^{\Omega(s)} H e^{-\Omega(s)} \\ &= H + [\Omega, H] = \frac{1}{2}[\Omega, [\Omega, H]] + \ldots \\ &= \sum_{k=0}^{\infty} \frac{1}{k!}[\Omega, H]^k \end{aligned}$$

$$\text{Flow eq. for } \Omega\text{:} \ \frac{d\Omega}{ds} = \sum_{k=0}^{\infty} \frac{B_k}{k!}[\Omega, \eta]^k$$

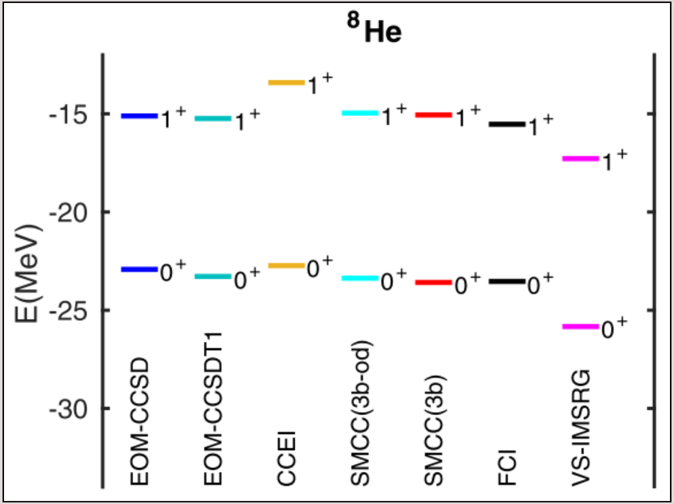
T.D. Morris PhD Thesis



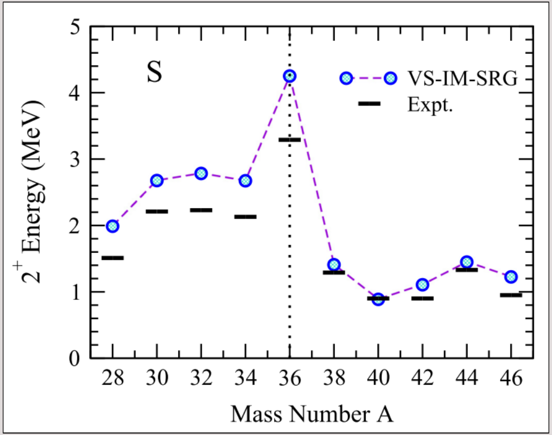
−100
−105
−110
−115
−120
−125
−130
−135
Energy (MeV)
0
5
10
15
20
Number of iterations n
^{16}O
$\langle \Phi_0 | \tilde{H} | \Phi_0 \rangle$
MBPT(2)
Experiment
MBPT(3)

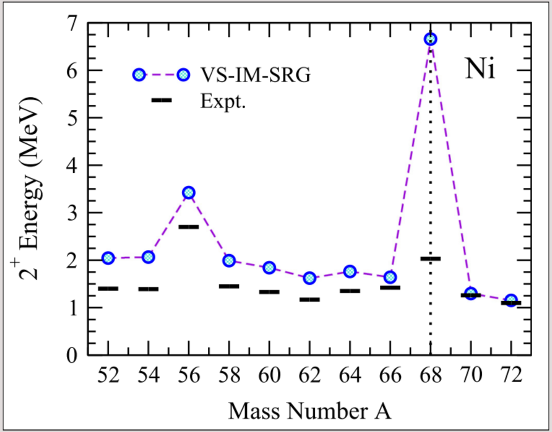


10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
$\|\tilde{H}_{od}/\Delta\|$
0
20
40
60
80
100
120
140
Number of iterations n
^{16}O
convergence threshold



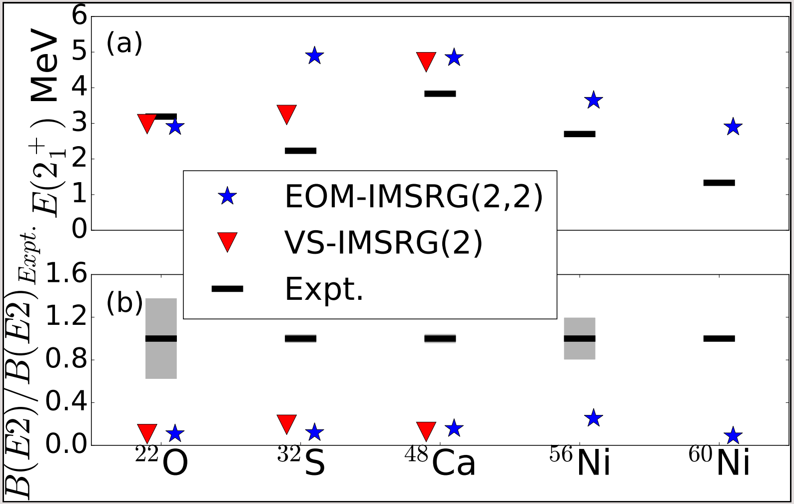
Sun et al. 2018



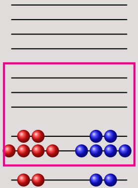


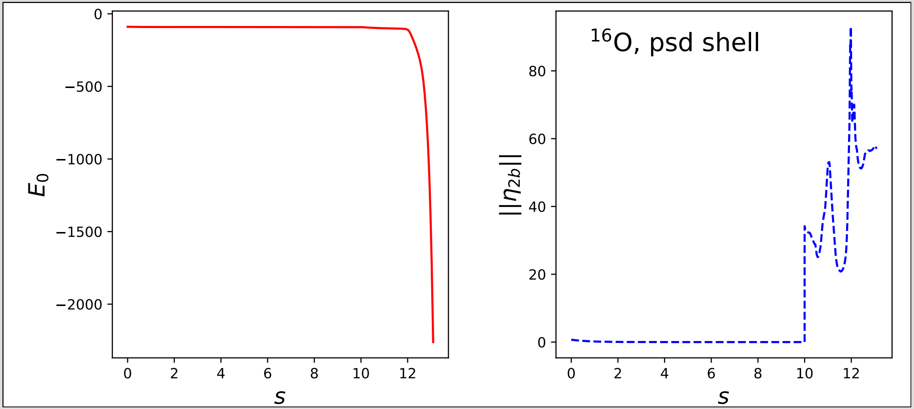
Simonis et al. 2017

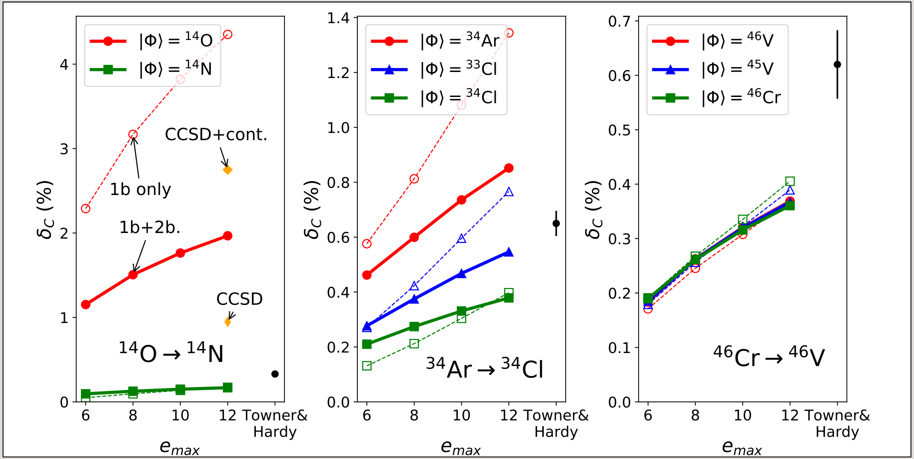
IMSRG(2) failings: $E2$ transitions



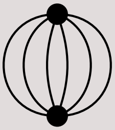
Parzuchowski et al. 2017



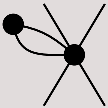
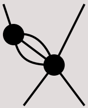
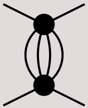

E_0
0
−500
−1000
−1500
−2000
s
0 2 4 6 8 10 12
^{16}O, psd shell
$||\eta_{2b}||$
0
20
40
60
80
s
0 2 4 6 8 10 12



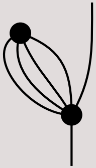
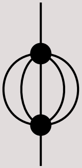
Gaute Hagen, priv. comm.

$\frac{d}{ds}E_0 =$ 

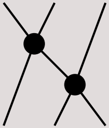
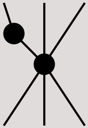
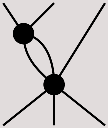
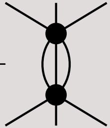
$[3,3]\to 0$ $\sim n^6$

$\frac{d}{ds}\Gamma =$  $+$  $+$ 

$[1,3]\to 2$ $\sim n^6$ | $[2,3]\to 2$ $\sim n^7$ | $[3,3]\to 2$ $\sim n^8$

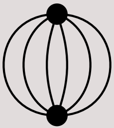
$\frac{d}{ds}f =$  $+$ 

$[2,3]\to 1$ $\sim n^6$ | $[3,3]\to 1$ $\sim n^7$

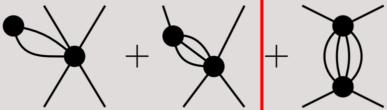
$\frac{d}{ds}W =$  $+$  $+$  $+$ 

$[2,2]\to 3$ $\sim n^7$ | $[1,3]\to 3$ $\sim n^7$ | $[2,3]\to 3$ $\sim n^8$ | $[3,3]\to 3$ $\sim n^9$

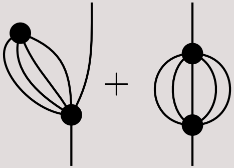
IMSRG(3) corrections to IMSRG(2) flow

$$\frac{d}{ds}E_0 =$$ 

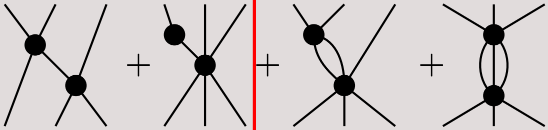
$[3,3]\!\rightarrow\!0$ $\sim n^6$

$$\frac{d}{ds}\Gamma =$$ 

$[1,3]\!\rightarrow\!2$ $\sim n^6$ | $[2,3]\!\rightarrow\!2$ $\sim n^7$ | $[3,3]\!\rightarrow\!2$ $\sim n^8$

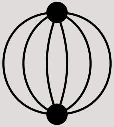
$$\frac{d}{ds}f =$$ 

$[2,3]\!\rightarrow\!1$ $\sim n^6$ | $[3,3]\!\rightarrow\!1$ $\sim n^7$

$$\frac{d}{ds}W =$$ 

$[2,2]\!\rightarrow\!3$ $\sim n^7$ | $[1,3]\!\rightarrow\!3$ $\sim n^7$ | $[2,3]\!\rightarrow\!3$ $\sim n^8$ | $[3,3]\!\rightarrow\!3$ $\sim n^9$

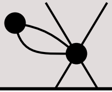
$$\frac{d}{ds}E_0 =$$



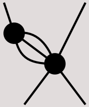
$[3,3]\rightarrow 0$

$\sim n^6$

$$\frac{d}{ds}\Gamma =$$



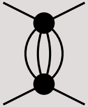
$+$



$[2,3]\rightarrow 2$

$\sim n^7$

$+$



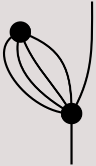
$[3,3]\rightarrow 2$

$\sim n^8$

Error, keeping only n^7 terms:

- $E_0 \sim$ 5th order
- $f \sim$ 4th order
- $\Gamma \sim$ 4th order
- $W \sim$ 3rd order

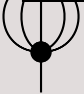
$$\frac{d}{ds}f =$$



$[2,3]\rightarrow 1$

$\sim n^6$

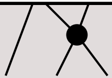
$+$



$[3,3]\rightarrow 1$

$\sim n^7$

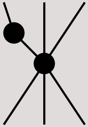
$$\frac{d}{ds}W =$$



$[2,2]\rightarrow 3$

$\sim n^7$

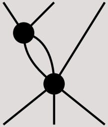
$+$



$[1,3]\rightarrow 3$

$\sim n^7$

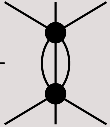
$+$



$[2,3]\rightarrow 3$

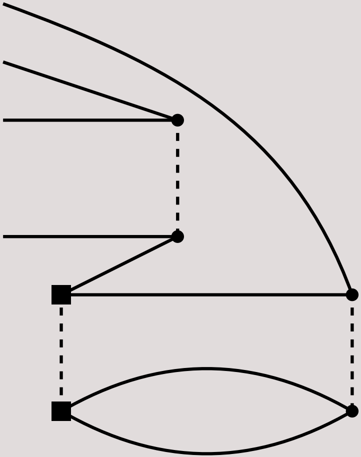
$\sim n^8$

$+$

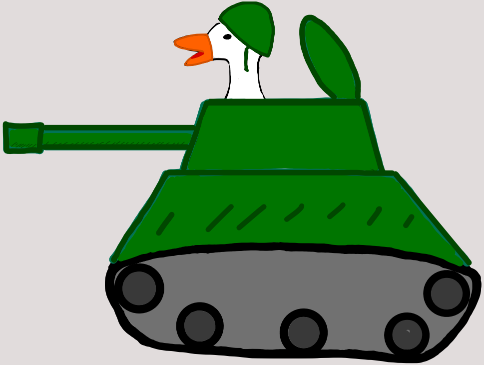


$[3,3]\rightarrow 3$

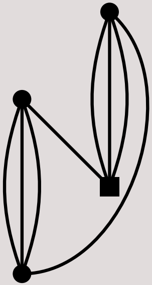
$\sim n^9$



$$[\Omega, [\Omega, H]_{3b}]_{2b}$$



T.D. Morris PhD Thesis



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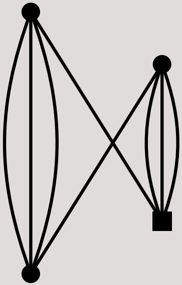
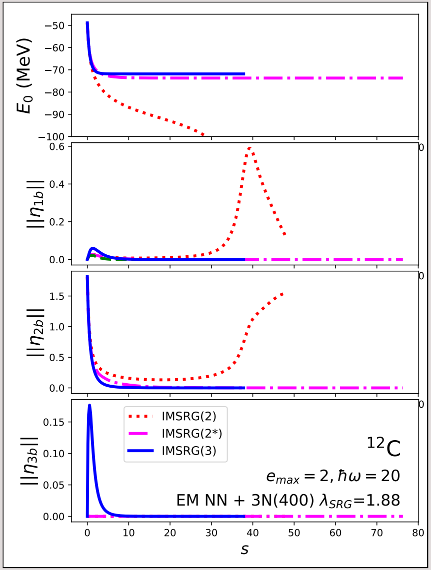


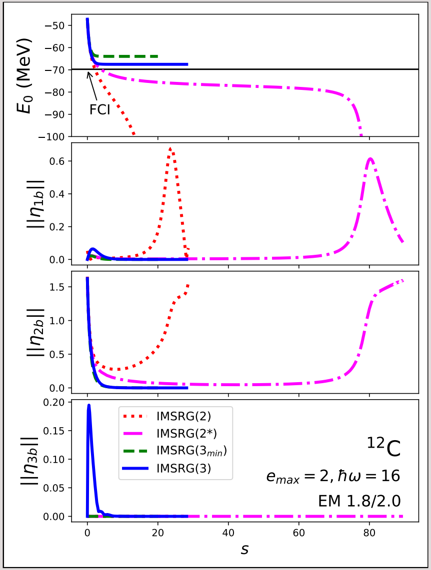
Included

Remedy: $[\Omega,[\Omega,H]] \rightarrow [\Omega,[\Omega,H]] + [\Omega,\chi]$ where $\chi =$ 

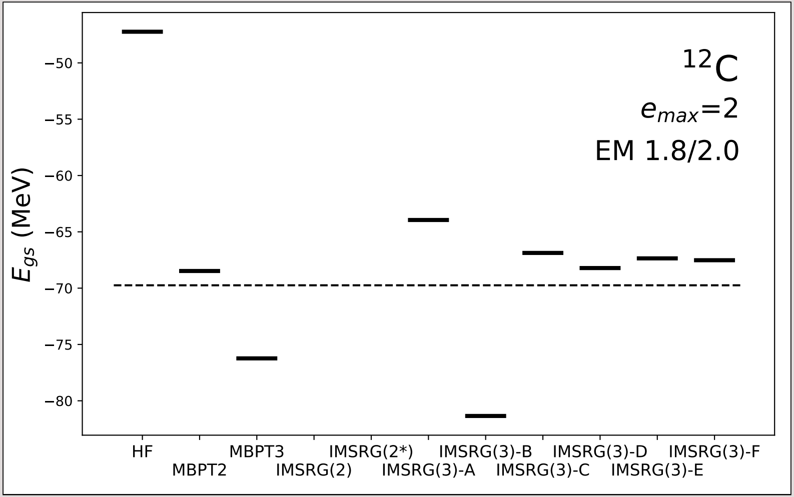
[IMSRG(2*) approx]



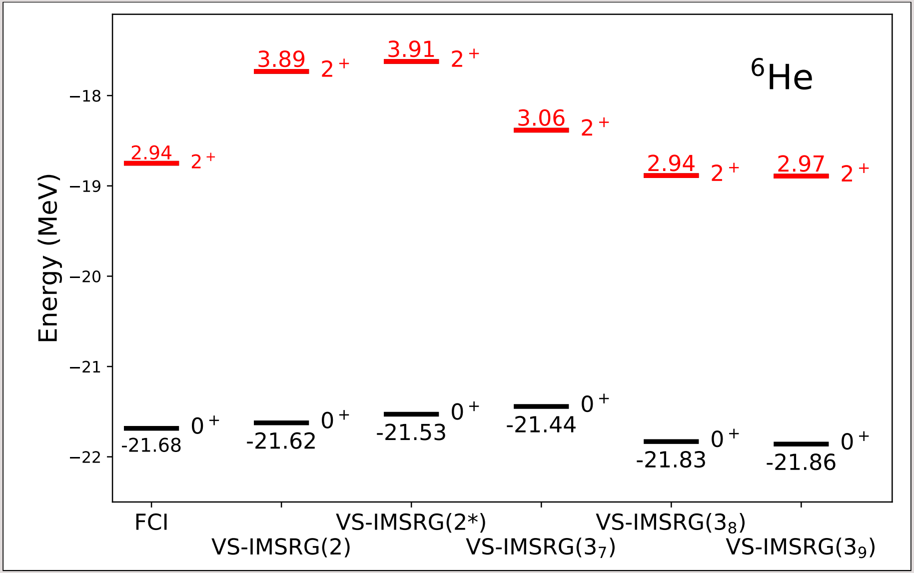
E_0 (MeV)
$||\eta_{1b}||$
$||\eta_{2b}||$
$||\eta_{3b}||$
IMSRG(2)
IMSRG(2*)
IMSRG(3)
^{12}C
$e_{max} = 2, \hbar\omega = 20$
EM NN + 3N(400) λ_{SRG}=1.88
s



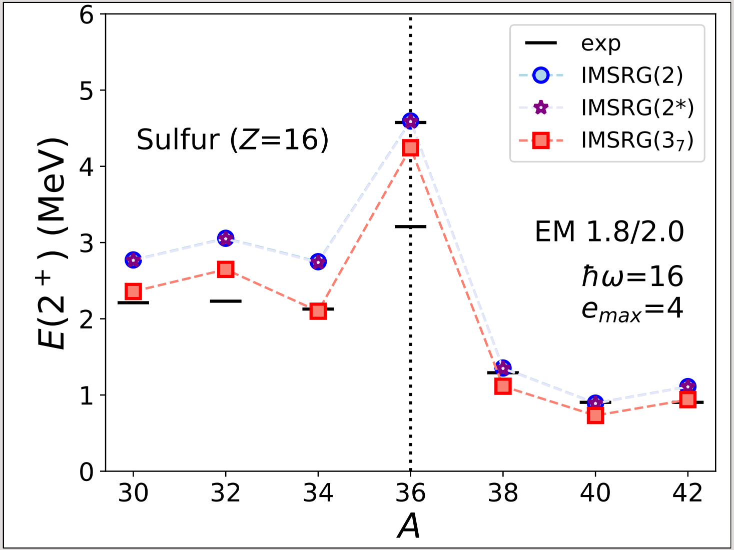
E_0 (MeV)
FCI
$||\eta_{1b}||$
$||\eta_{2b}||$
$||\eta_{3b}||$
IMSRG(2)
IMSRG(2*)
IMSRG(3_{min})
IMSRG(3)
^{12}C
$e_{max} = 2, \hbar\omega = 16$
EM 1.8/2.0
s



- A: $[2,2] \rightarrow 3$ + $[2,3] \rightarrow 2$, η_{2b},Ω_{2b}
- B: A + η_{3b},Ω_{3b}
- C: B + $[1,3] \rightarrow 3$
- D: C + $[3,3] \rightarrow 0$
- E: D + $[2,3] \rightarrow 1$
- F: E + $[1,3] \rightarrow 2$



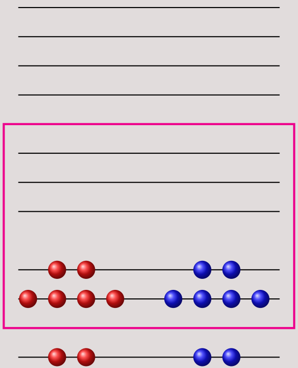
^{6}He
Energy (MeV)
−18
−19
−20
−21
−22
2.94 2^+
3.89 2^+
3.91 2^+
3.06 2^+
2.94 2^+
2.97 2^+
-21.68 0^+
-21.62 0^+
-21.53 0^+
-21.44 0^+
-21.83 0^+
-21.86 0^+
FCI
VS-IMSRG(2)
VS-IMSRG(2*)
VS-IMSRG(3_7)
VS-IMSRG(3_8)
VS-IMSRG(3_9)

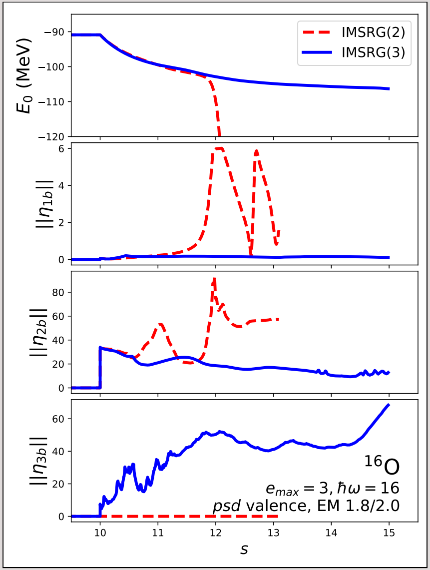


IMSRG(3_7) calculations made with cut

$\tilde{e}_a + \tilde{e}_b + \tilde{e}_c \leqslant \tilde{E}_{max} = 2$,

$\tilde{e}_a \equiv 2n_a + \ell_a - \epsilon_F$




IMSRG(2)
IMSRG(3)
E_0 (MeV)
$||\eta_{1b}||$
$||\eta_{2b}||$
$||\eta_{3b}||$
s
^{16}O
$e_{max} = 3, \hbar\omega = 16$
psd valence, EM 1.8/2.0

Summary

- 3-body contributions can help stabilize IMSRG flow (e.g. ^{12}C), and improve excitation energies
- Multi-shell decoupling leads to rapid growth of 3-body terms and loss of cluster hierarchy. Keeping 3 body terms is no help.
- Main effects appear to come from n^7 scaling terms
- To do:
  - Optimize, factorize nested commutator terms to n^6
  - How best to use IMSRG(3) to assess uncertainty?

Thanks to Titus Morris, Takayuki Miyagi, Julien Ripoche, Alex Tichai, and Roland Wirth for helpful discussions.

Additional figures

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