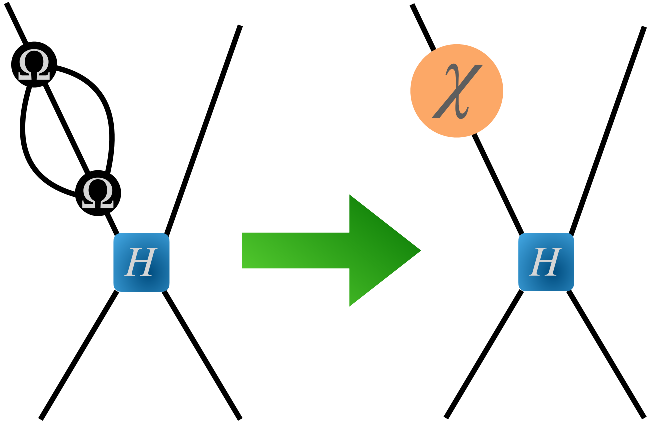
# Factorized Approximations of IMSRG(3)

## or **How to make $n^9$ money for $n^6$ effort**




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

Ragnar Stroberg
University of Notre Dame

PAINT24
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TRIUMF, Vancouver, BC

Work done in collaboration with
**Bingcheng He** and Titus Morris

# IMSRG (Magnus formulation)

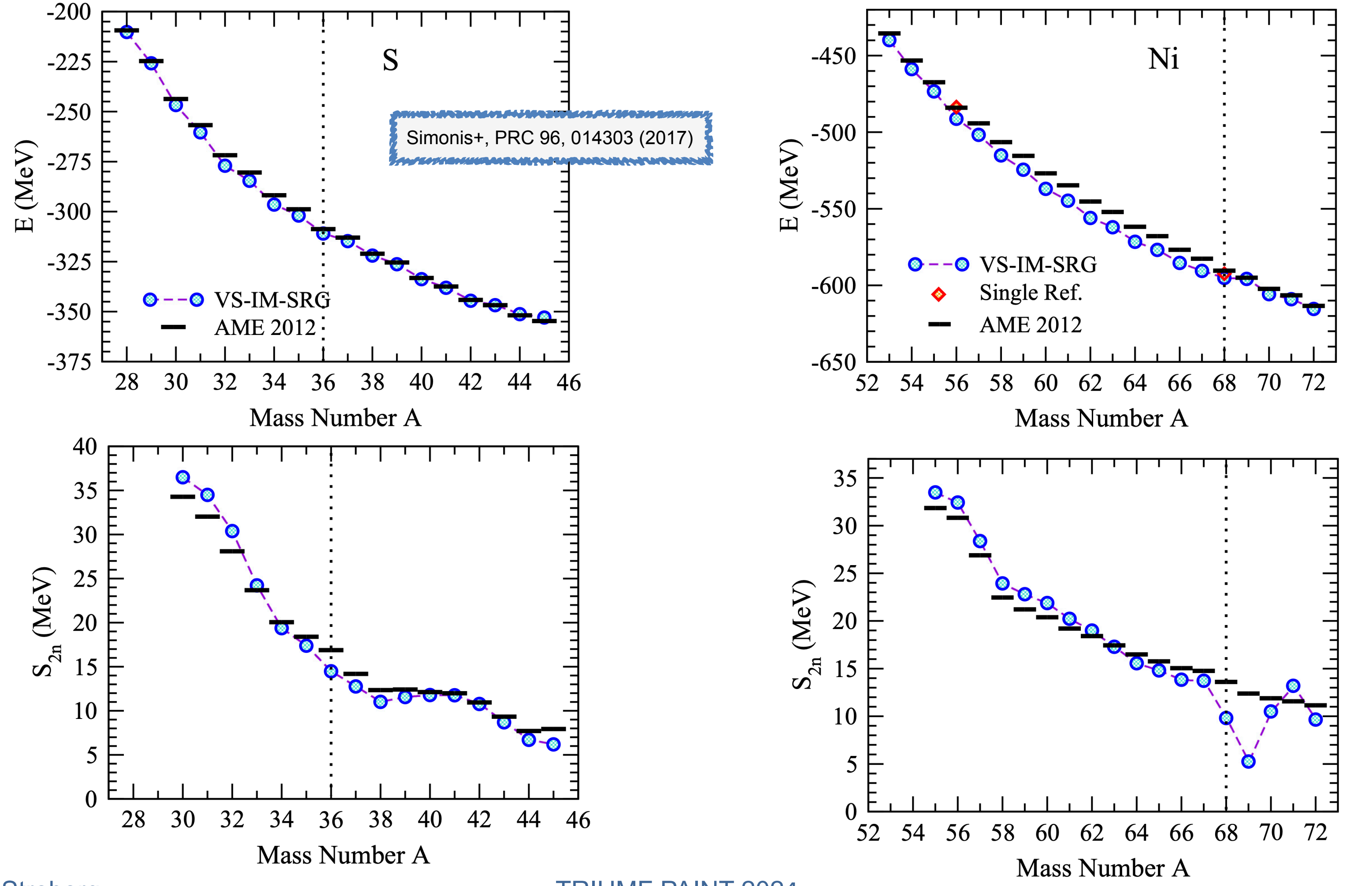
$$H(s) = e^{\Omega(s)} H(0) e^{-\Omega(s)}$$

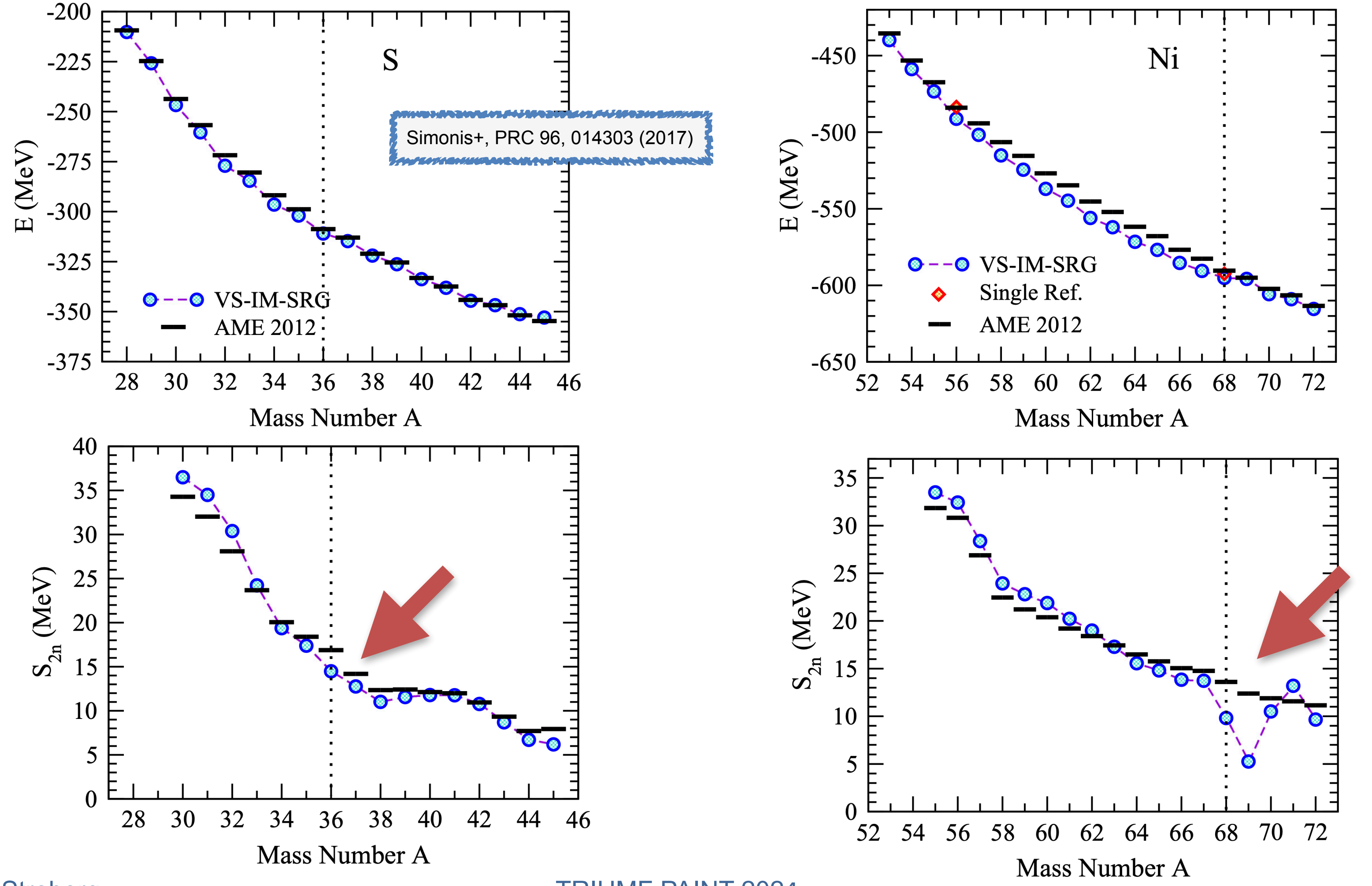
$$= H + [\Omega, H] + \frac{1}{2!}\left[\Omega, [\Omega, H]\right] + \dots$$

$$\frac{d}{ds}\Omega = \sum_k \frac{B_k}{k!}[\eta, \Omega]^{(k)}$$

IMSRG(2): Truncate all operators at 2b level

$$\left[\Omega, [\Omega, H]\right] \rightarrow \left[\Omega_{2b}, [\Omega_{2b}, H_{2b}]_{2b}\right]_{2b}$$


S
Ni
Simonis+, PRC 96, 014303 (2017)
VS-IM-SRG
AME 2012
Single Ref.
E (MeV)
$S_{2n}$ (MeV)
Mass Number A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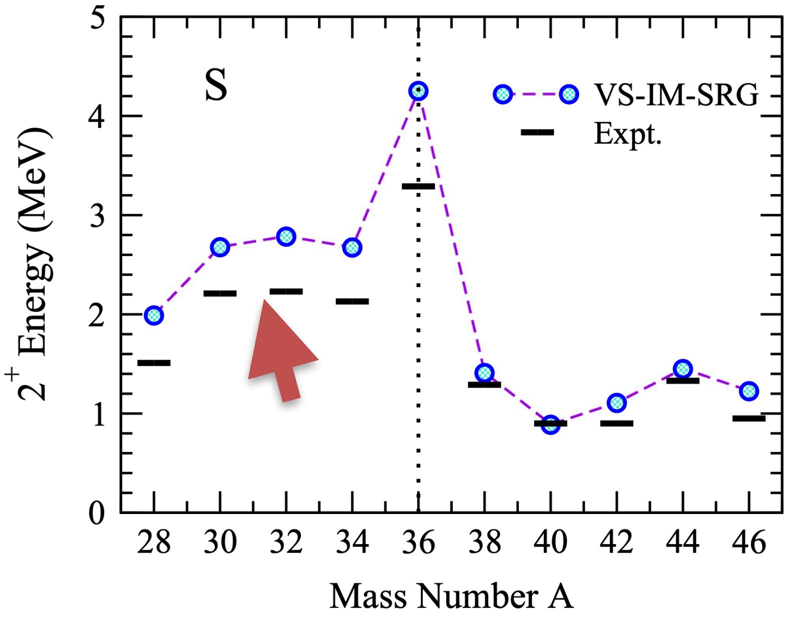
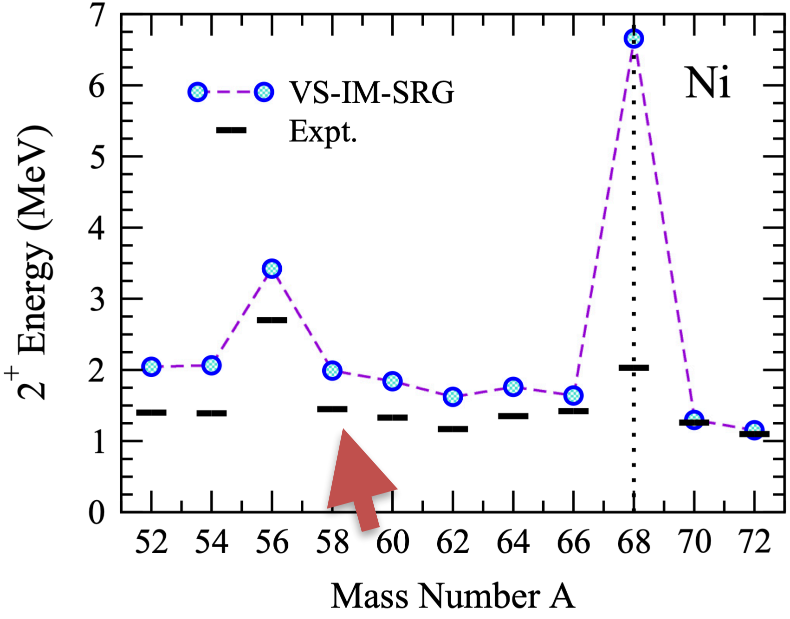


S
VS-IM-SRG
Expt.
2+ Energy (MeV)
Mass Number A

Ni
VS-IM-SRG
Expt.
2+ Energy (MeV)
Mass Number A

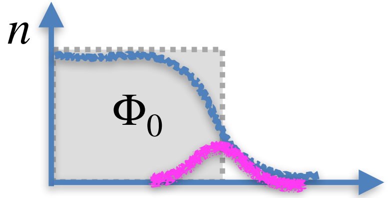
# Can IMSRG(3) fix this?

# Naive Dimensionless Analysis

## Normal ordering:

$$\hat{V}^{3N} \rightarrow \frac{1}{3!}\sum_{abc} \rho_a \rho_b \rho_c V_{abcabc} + \frac{1}{2!}\sum_{ab} \rho_a \rho_b V_{iablab}\{a_i^\dagger a_l\} + \sum_a \rho_a V_{ijalma}\{a_i^\dagger a_j^\dagger a_m a_l\} + V_{ijklmn}\{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}$$

$$\langle V^{3N} \rangle \sim A^3 + A^2 n_{QP} + A n_{QP}^2 + n_{QP}^3$$



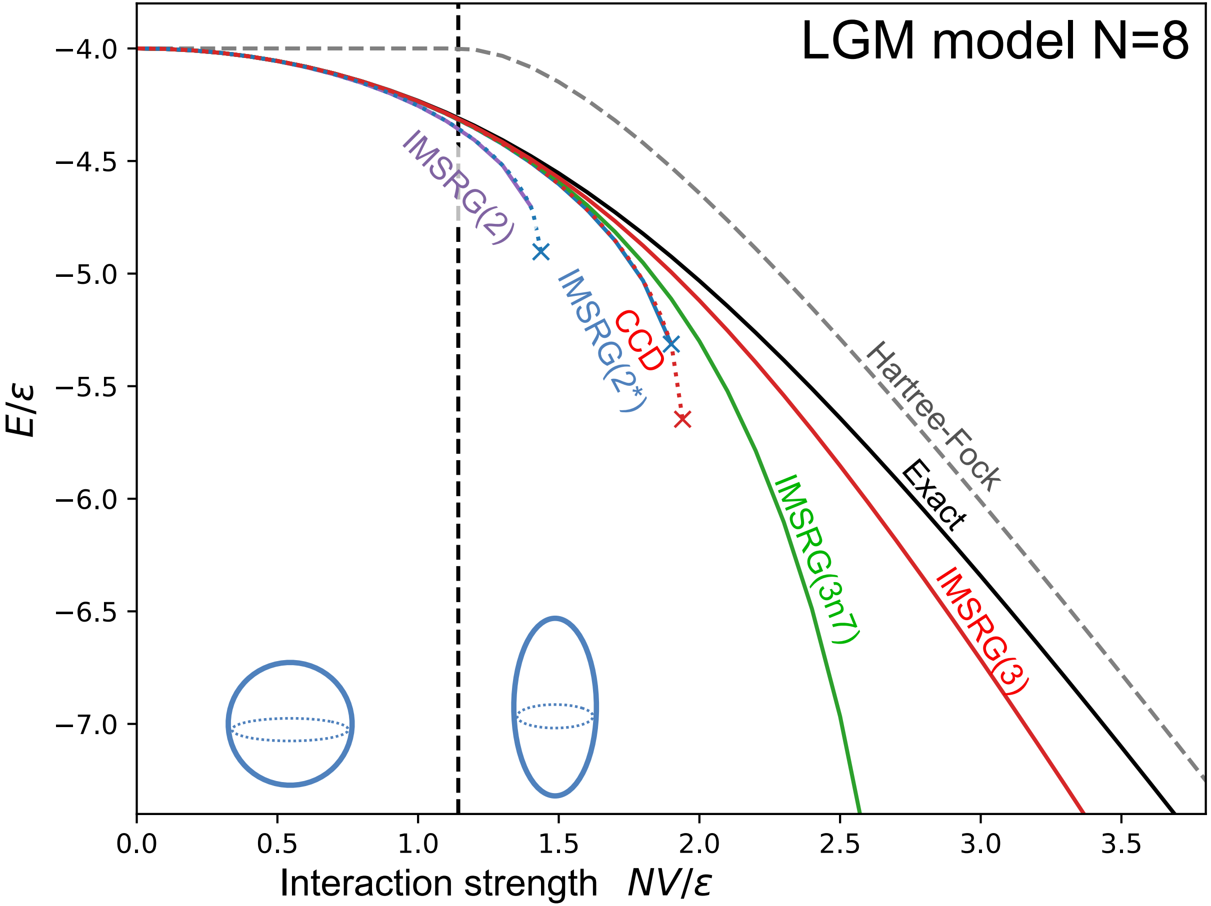

Increasing particle rank suppressed by powers of $\frac{n_{QP}}{A}$ **when evaluated in wave function**.

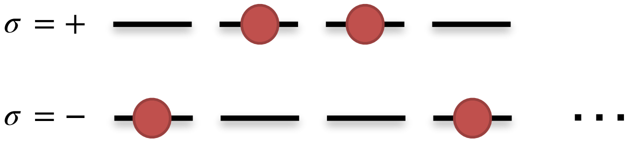
see e.g. Friman & Schwenk, "Three-body interactions in Fermi systems" 2011

Conjecture:

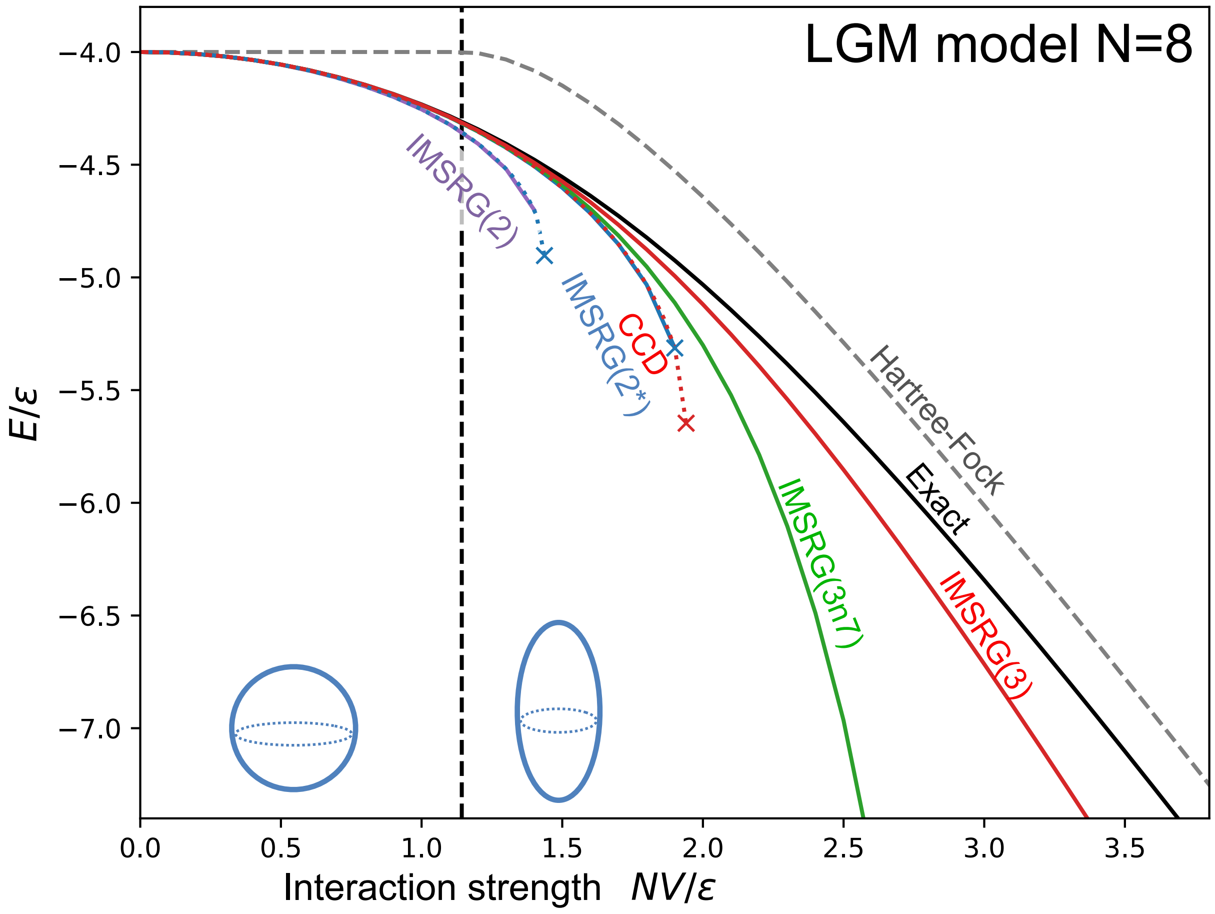
"Genuine" induced 3N forces are relatively unimportant. The main effect of 3N operators is as an **intermediate** which subsequently modifies 0b,1b,2b forces.

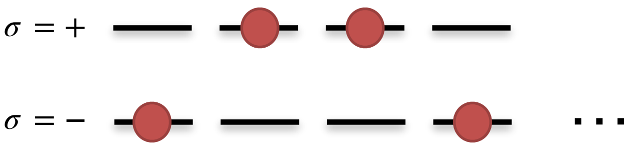
e.g. $$\left[\Omega_{\mathrm{2b}}, [\Omega_{\mathrm{2b}}, H_{\mathrm{2b}}]_{\mathrm{3b}}\right]_{\mathrm{1b,2b}}$$




$$H = \epsilon \sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma} - \frac{1}{2} V \sum_{pq} a^\dagger_{p+} a^\dagger_{q+} a_{q-} a_{p-} + h\,c$$

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By symmetry of LGM,
CCD = CCSDT
but
IMSRG(2) ≠ IMSRG(3)

Intermediate 3N operators are clearly important!

$$e^{\Omega} H e^{-\Omega} = H + [\Omega, H] + \frac{1}{2!}\left[\Omega, [\Omega, H]\right] + \dots$$

$$\left[\Omega_{2b}, [\Omega_{2b}, H_{2b}]_{3b}\right]_{1b,2b}$$

$$e^{\Omega}He^{-\Omega} = H + [\Omega, H] + \frac{1}{2!}\left[\Omega, [\Omega, H]\right] + \ldots$$

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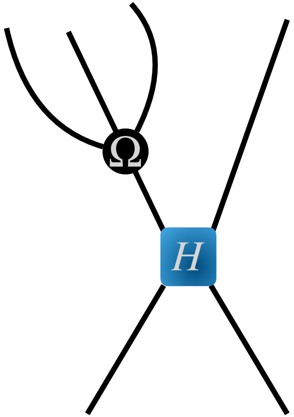

$[\Omega_{2b}, H_{2b}]_{3b}$

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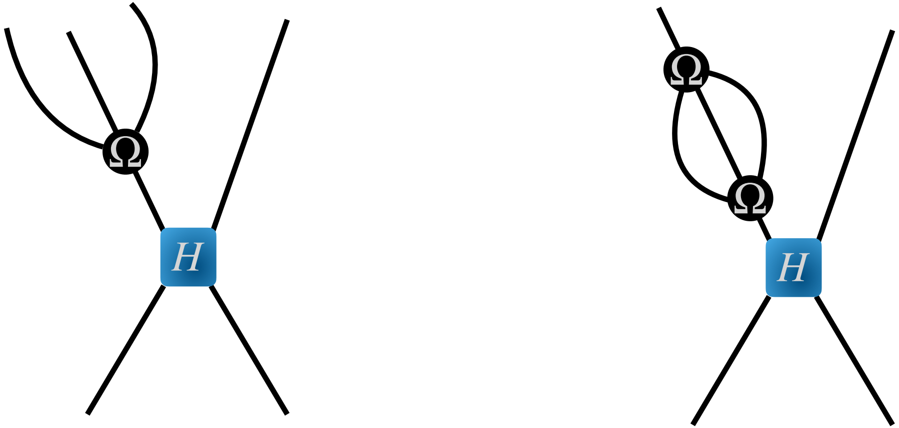


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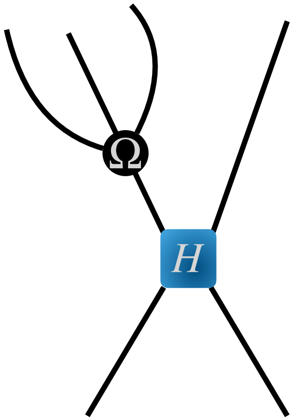


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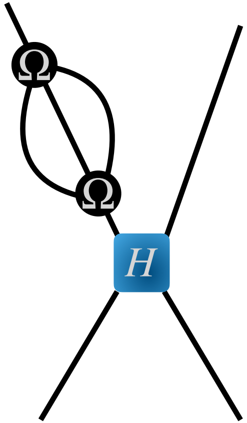
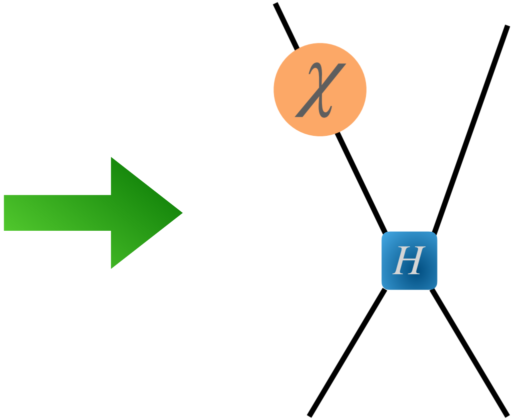



$\left[\Omega_{2b}, [\Omega_{2b}, H_{2b}]_{3b}\right]_{2b}$



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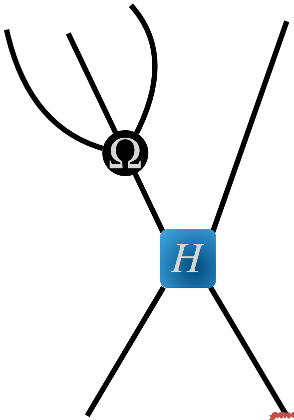
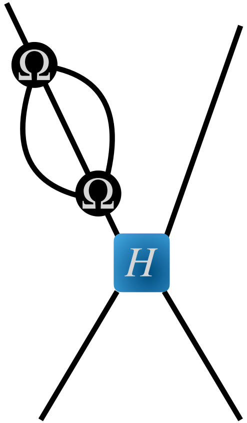
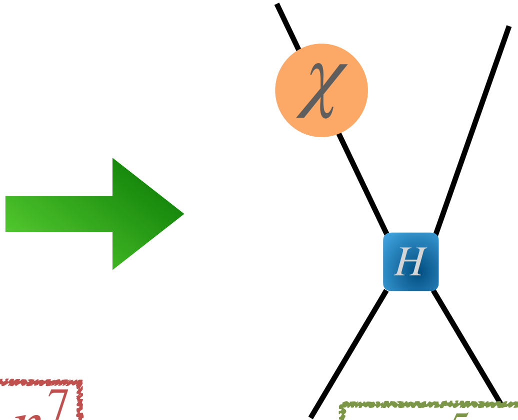


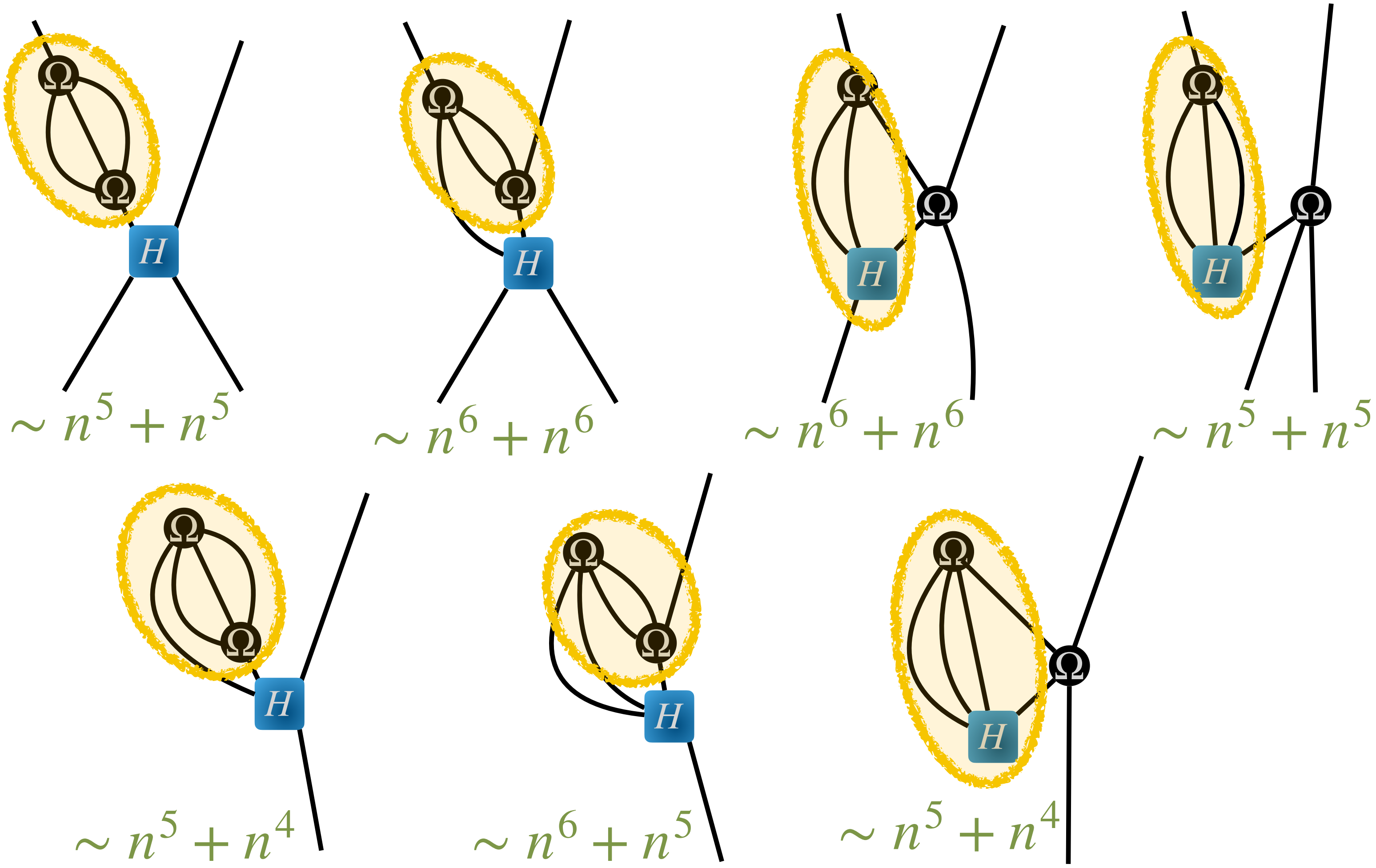

$[\Omega_{2b}, H_{2b}]_{3b}$ $\sim n^7$



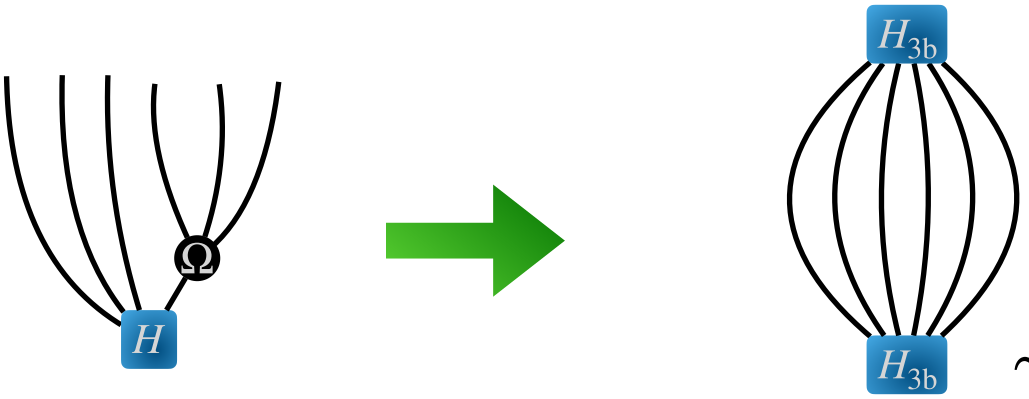

$\left[\Omega_{2b},[\Omega_{2b},H_{2b}]_{3b}\right]_{2b}$ $\sim n^7 + n^7$




$\sim n^5 + n^5$


Ω
H
$\sim n^5 + n^5$
$\sim n^6 + n^6$
$\sim n^6 + n^6$
$\sim n^5 + n^5$
$\sim n^5 + n^4$
$\sim n^6 + n^5$
$\sim n^5 + n^4$

# Leading genuine 3N force in 2nd order PT*




$\sim n^7 \sim n_h^3 n_p^4$

Arises from $\left[\Omega_{3b}, [\Omega_{2b}, H_{2b}]_{3b}\right]_{0b}$

*This can get formally messy for VS-IMSRG, but cavalierly using an ensemble reference $|\Phi_0\rangle$ captures the main effect pretty well.

# Introducing IMSRG(3f)

IMSRG(3f) $\equiv$ IMSRG(2)

$+\left[\Omega, [\Omega, H]_{3b}\right]_{1b,2b}$ w/ 1b intermediates during IMSRG flow

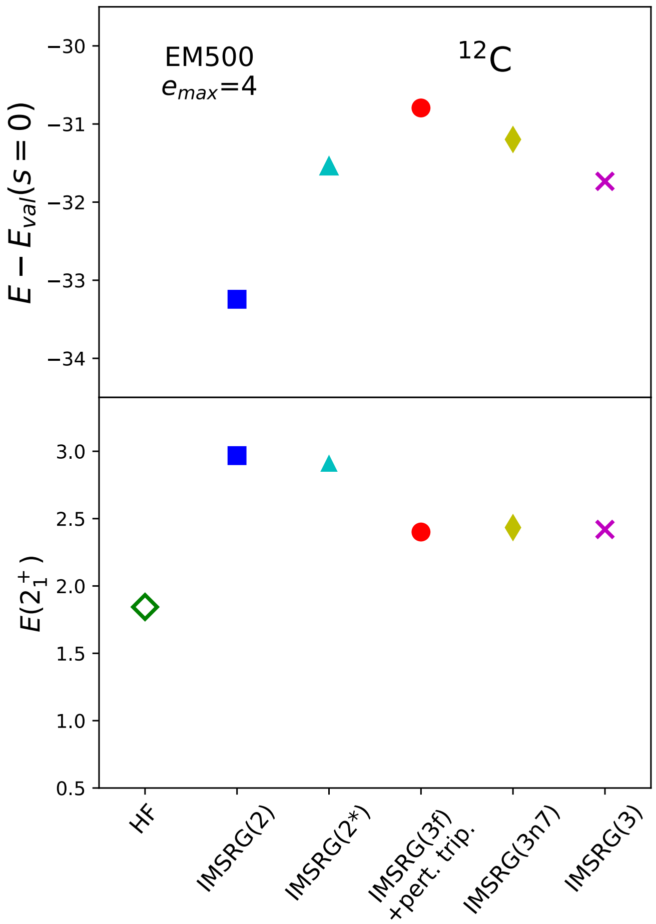
$+\left[\Omega, [\Omega, H]_{3b}\right]_{1b,2b}$ w/ 2b intermediates at $s = \infty$

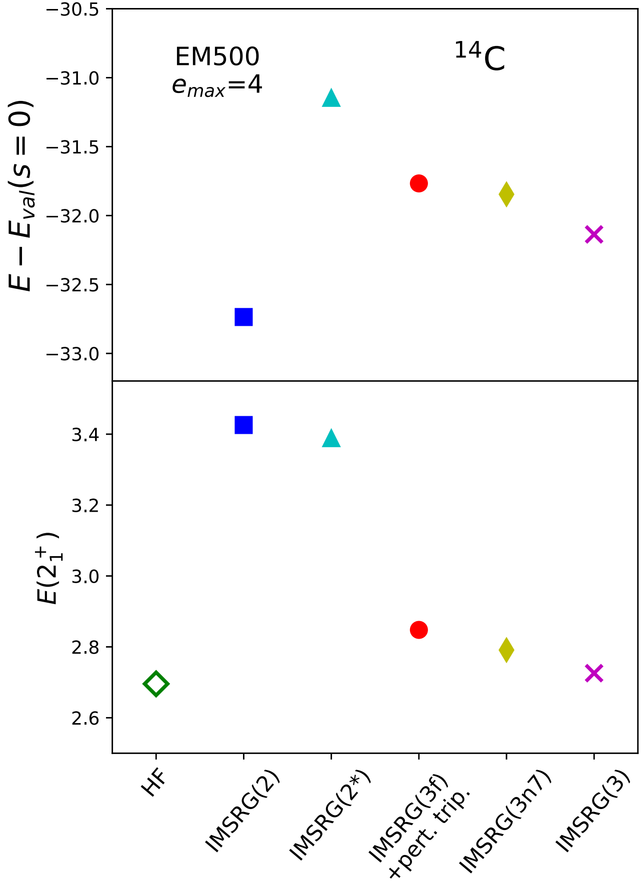
Perturbative triples = $[\Omega^{\text{pert}}_{3b}, H_{3b}]_{0b}$ at $s = \infty$

For LGM model, IMSRG(3f) reproduces IMSRG(3n7) exactly

Implementation of these corrections was aided immensely by the `amc` code
A. Tichai, R. Wirth, J. Ripoche, T. Duguet arXiv:2002.05011

# VS-IMSRG p-shell (NN only)



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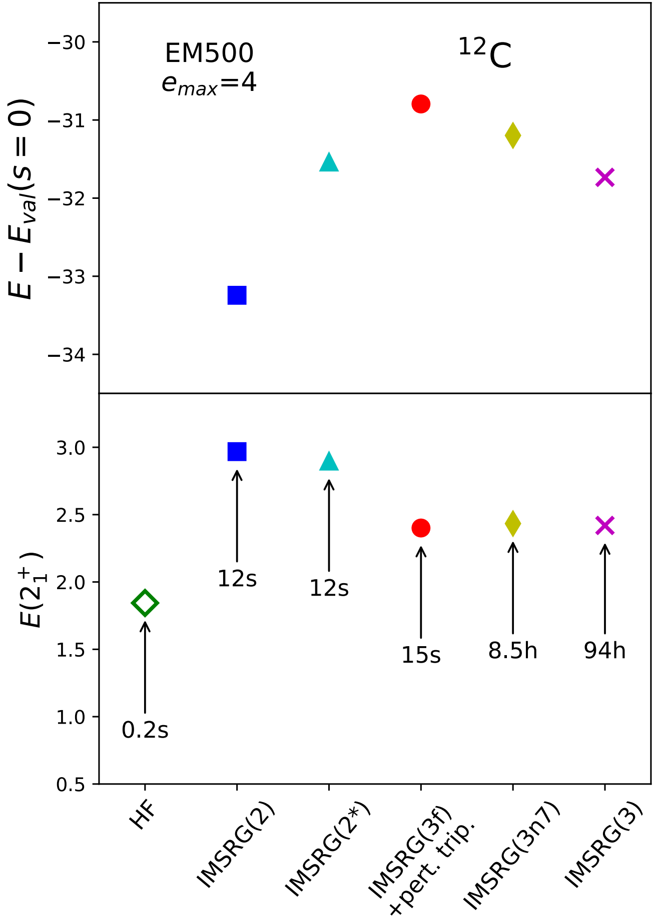
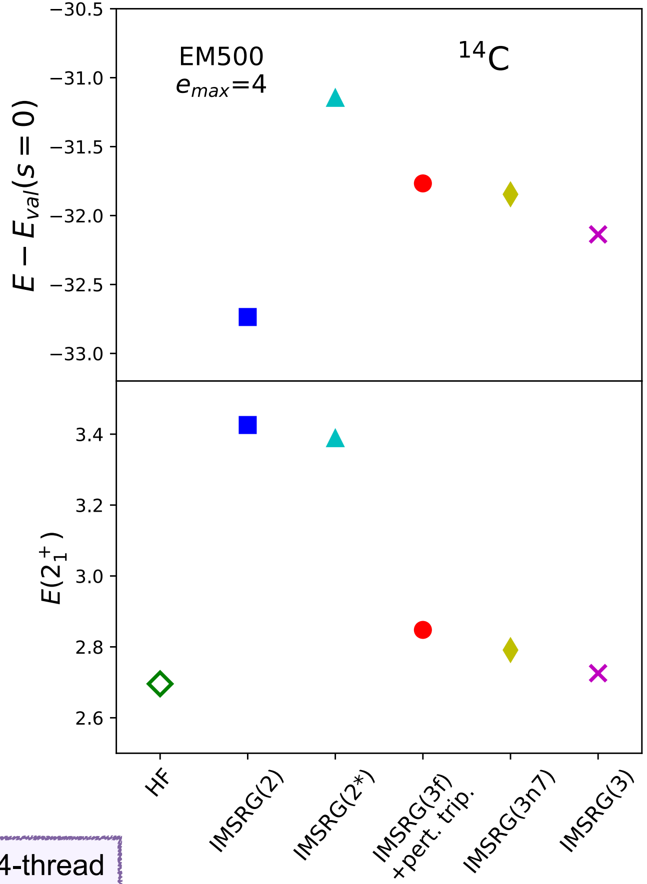
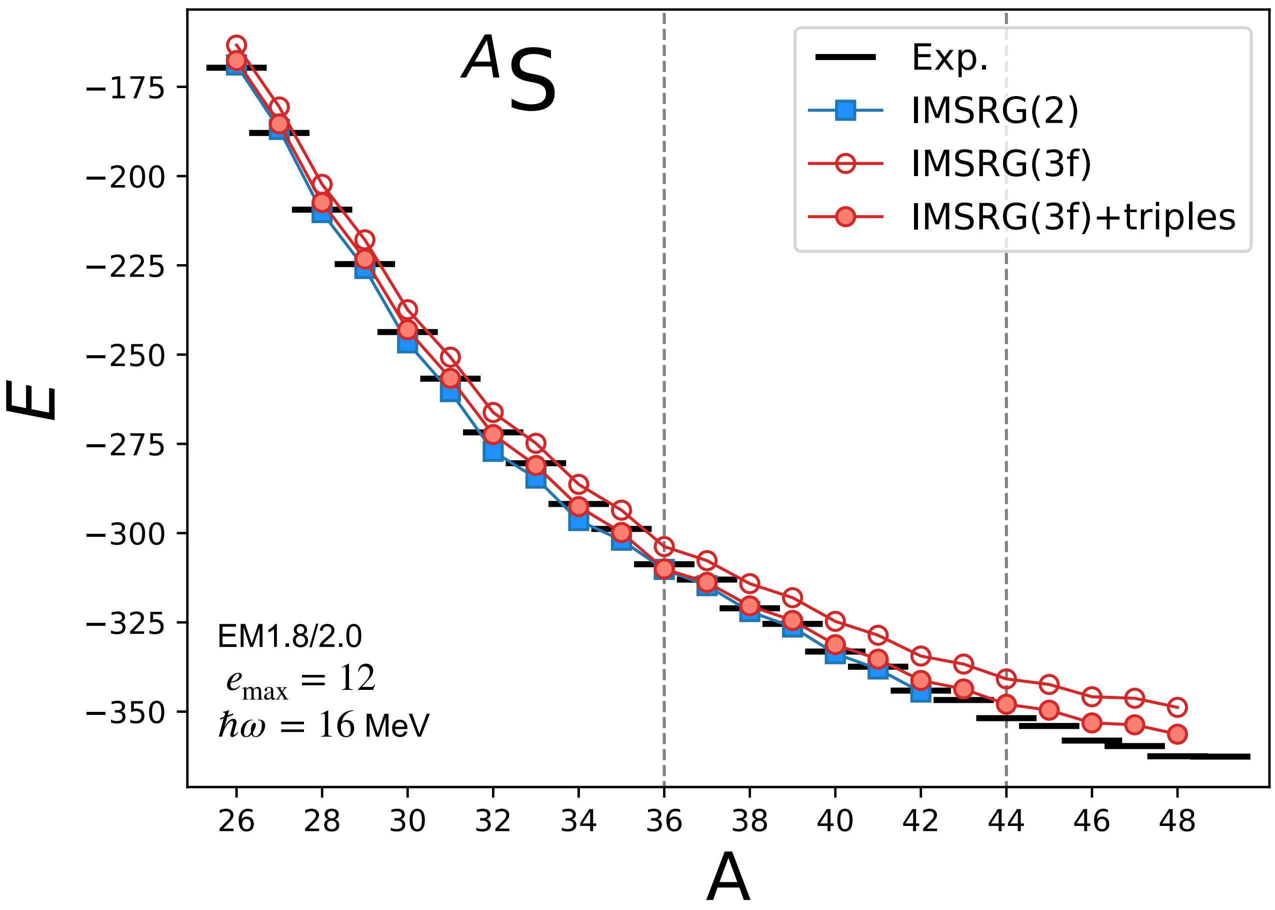
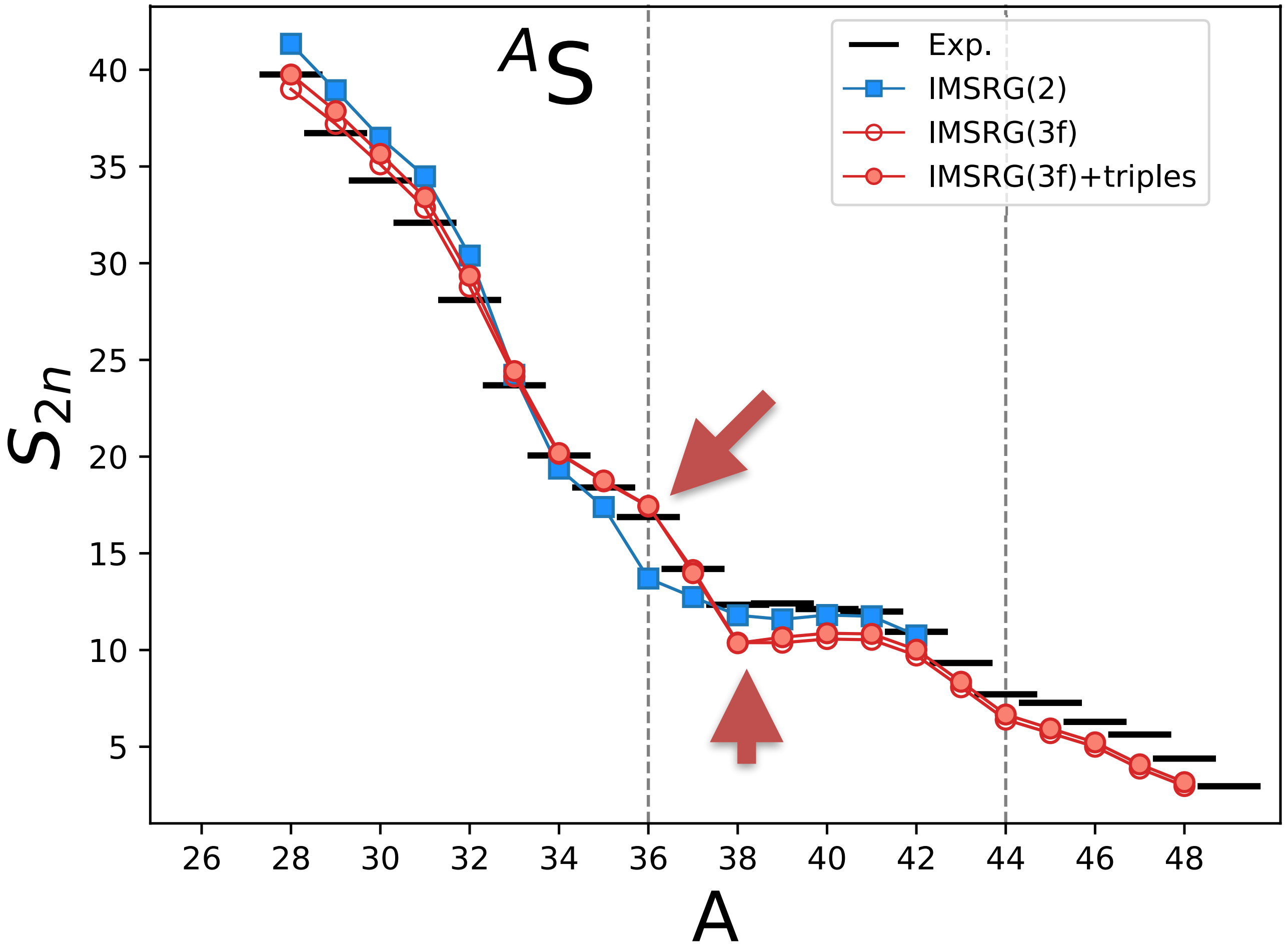


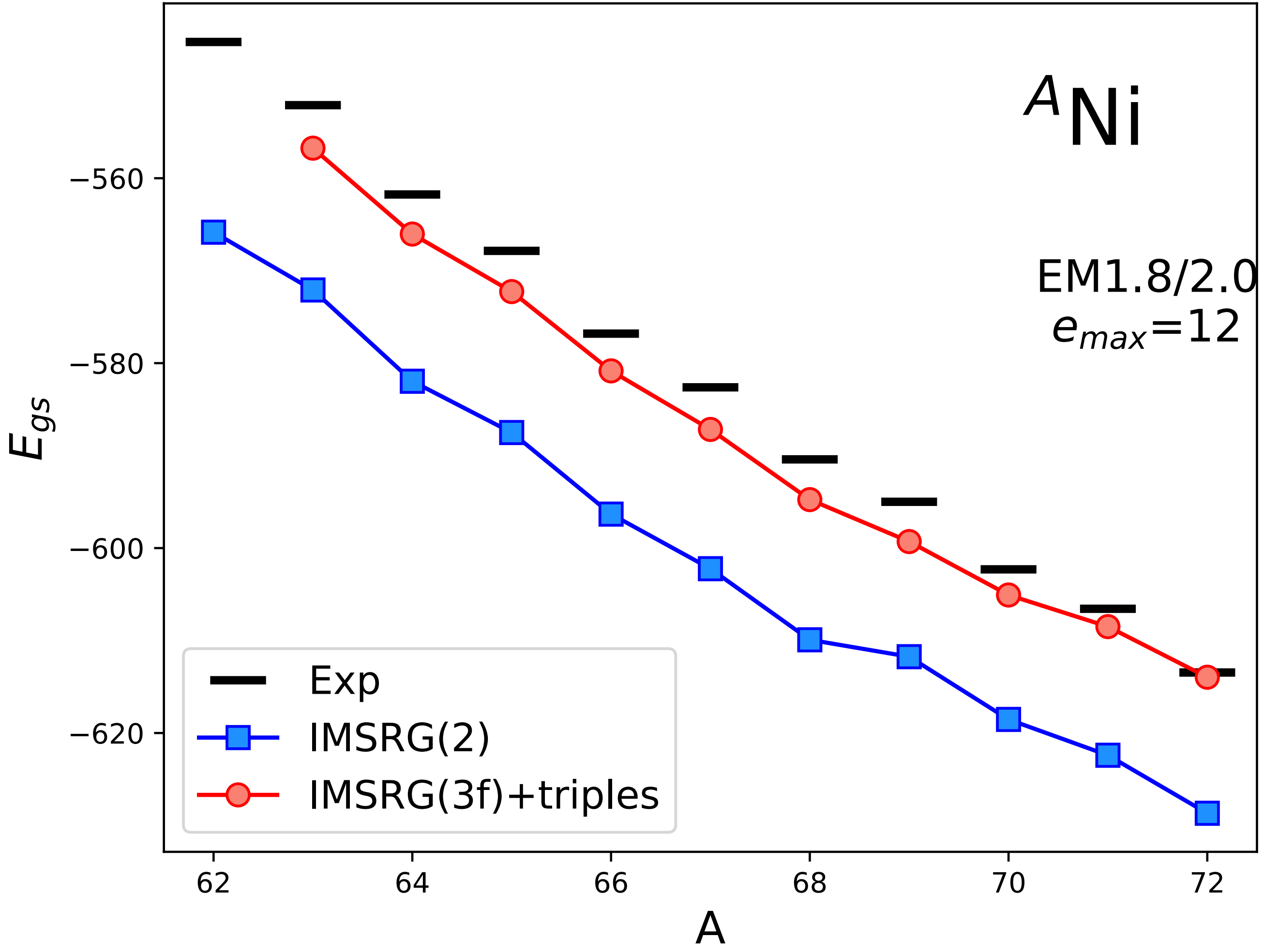

Compute times on 64-thread single node on CRC@ND



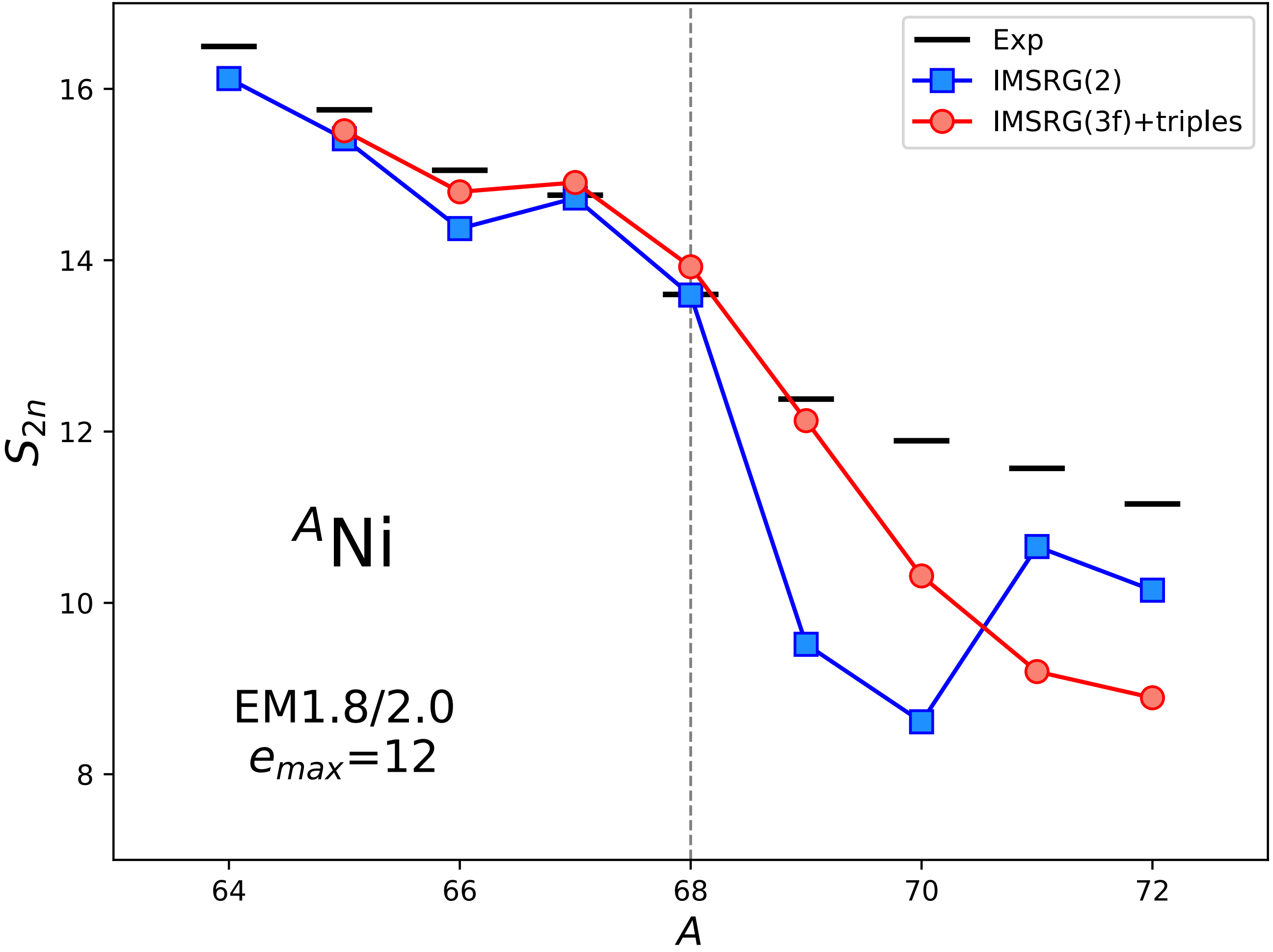
$^{A}$S
Exp.
IMSRG(2)
IMSRG(3f)
IMSRG(3f)+triples
EM1.8/2.0
$e_{max} = 12$
$\hbar\omega = 16$ MeV
E
A
−175
−200
−225
−250
−275
−300
−325
−350
26
28
30
32
34
36
38
40
42
44
46
48



$^{A}$S
$S_{2n}$
A
Exp.
IMSRG(2)
IMSRG(3f)
IMSRG(3f)+triples
40
35
30
25
20
15
10
5
26
28
30
32
34
36
38
40
42
44
46
48

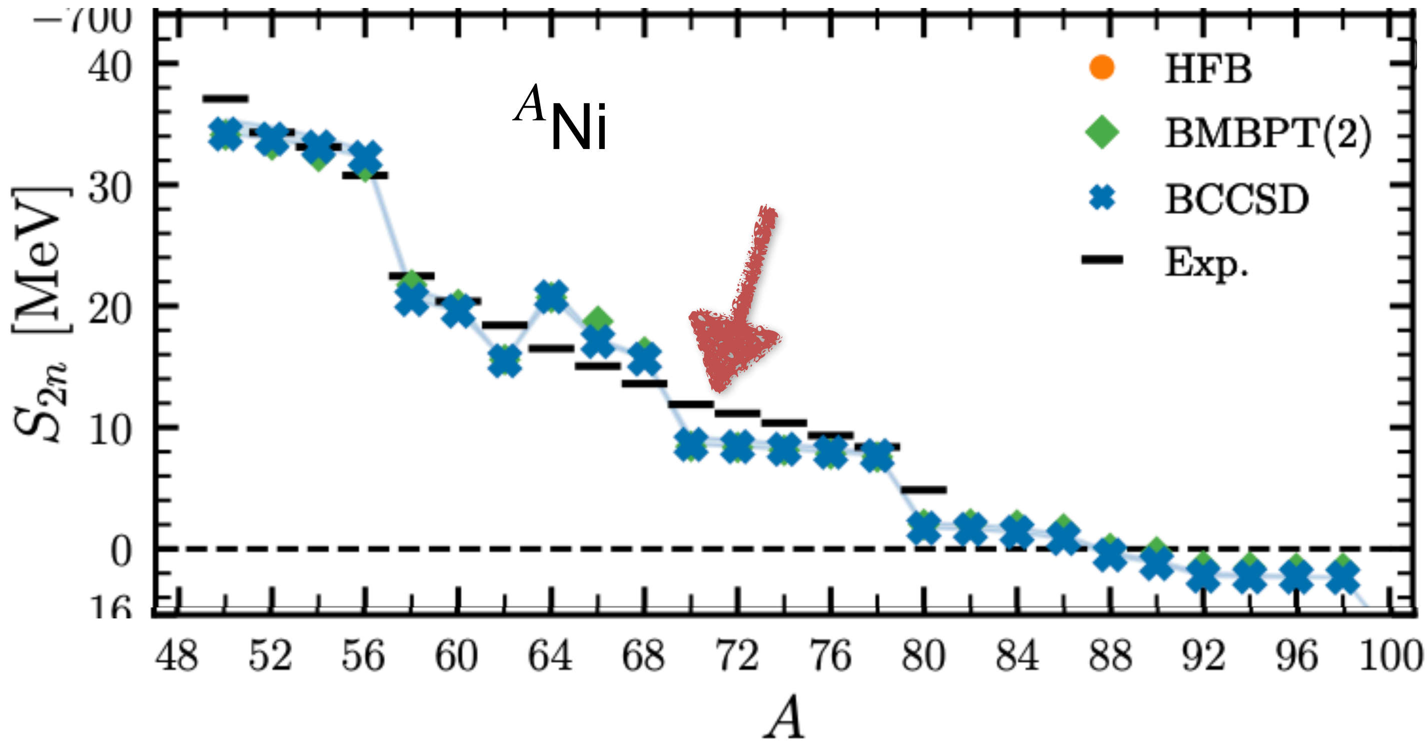


$^A$Ni
EM1.8/2.0
$e_{max}$=12
$E_{gs}$
A
−560
−580
−600
−620
62
64
66
68
70
72
Exp
IMSRG(2)
IMSRG(3f)+triples

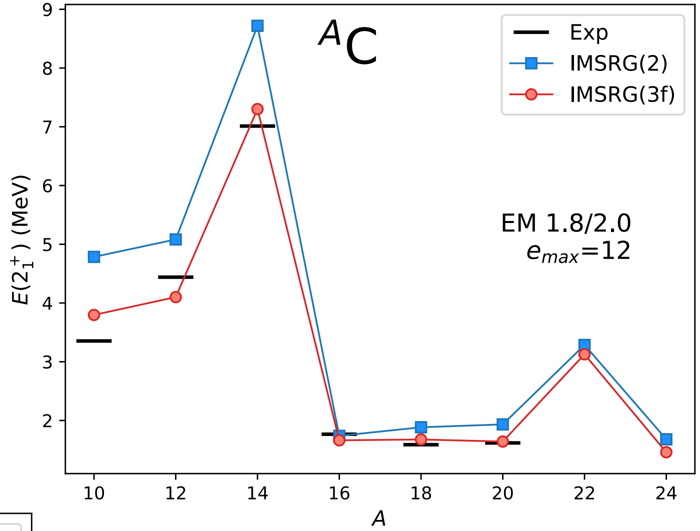


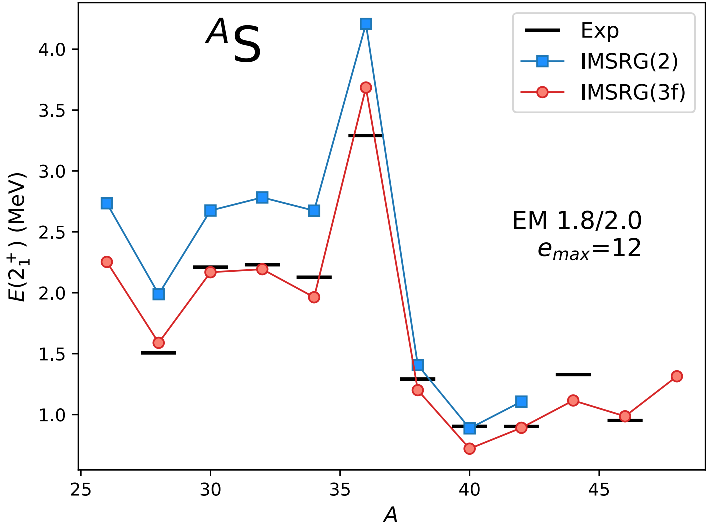
Exp
IMSRG(2)
IMSRG(3f)+triples
$S_{2n}$
16
14
12
10
8
$^{A}$Ni
EM1.8/2.0
$e_{max}$=12
64
66
68
70
72
$A$

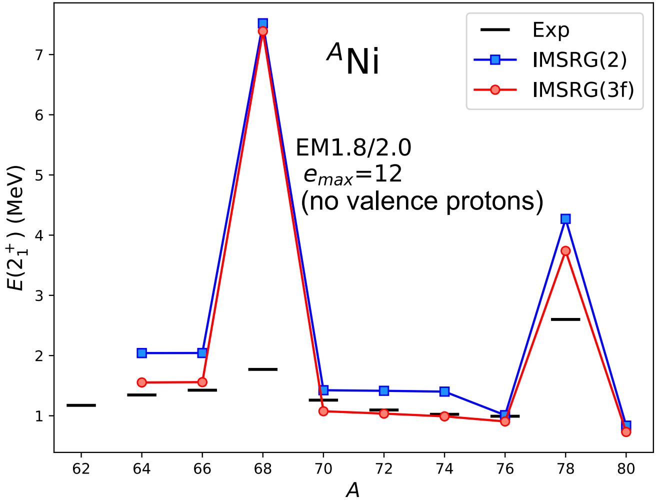
Tichai, Demol, Duguet arXiv:2307.15619



# 2+ Excitation energies

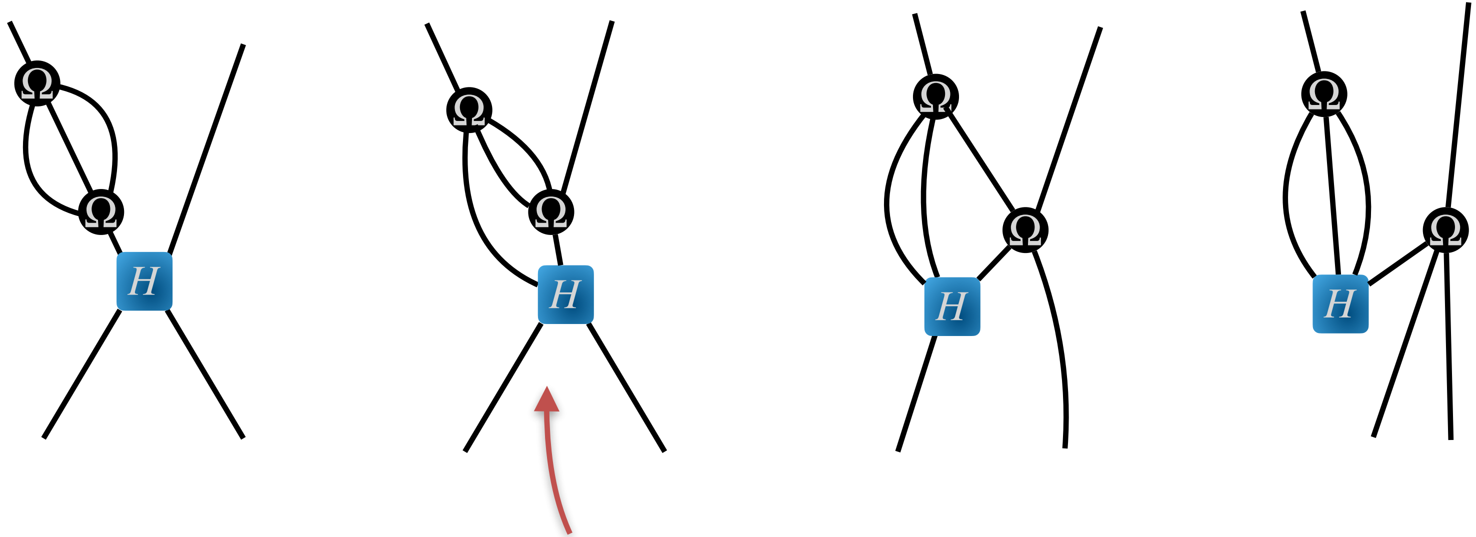


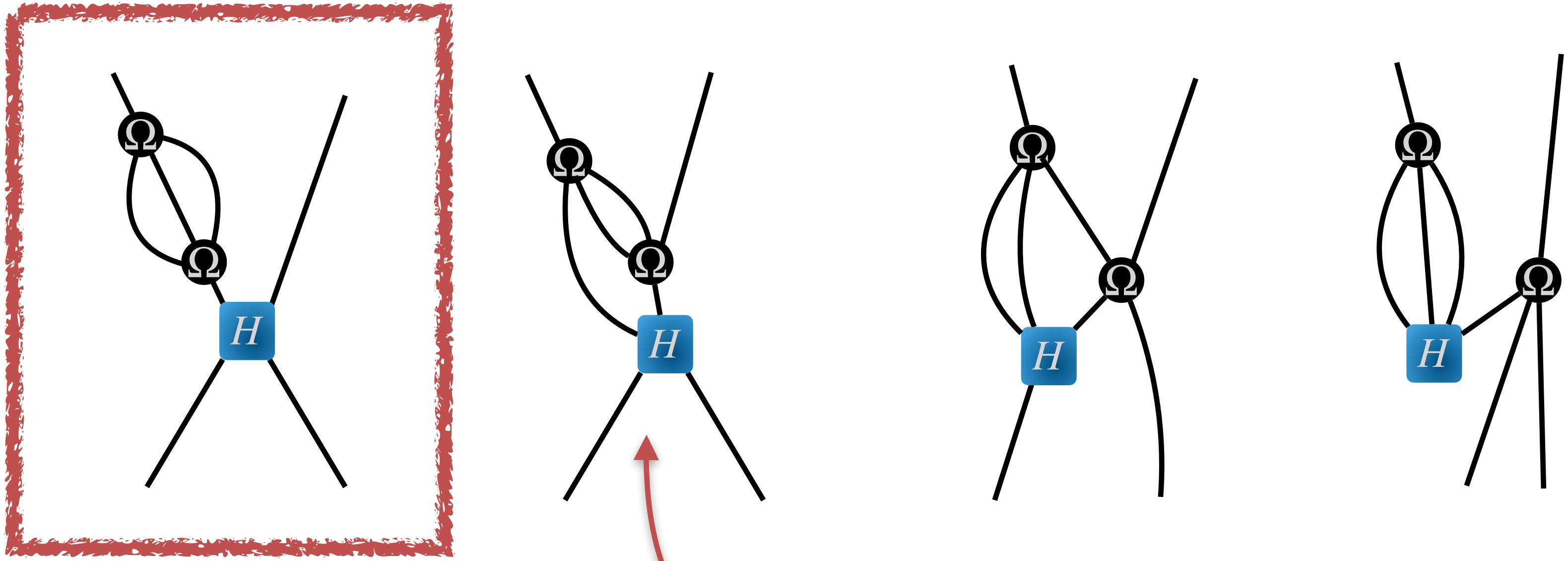
# A peek under the hood

# Not all diagrams contribute equally



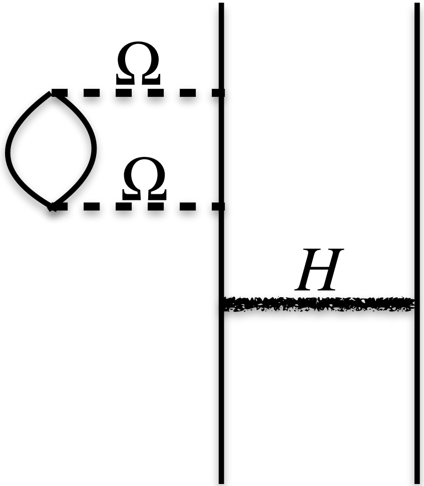

Also important for realistic potentials

# Not all diagrams contribute equally

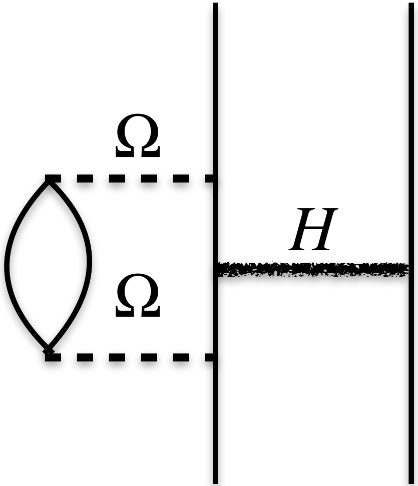



Dominant

Also important for realistic potentials

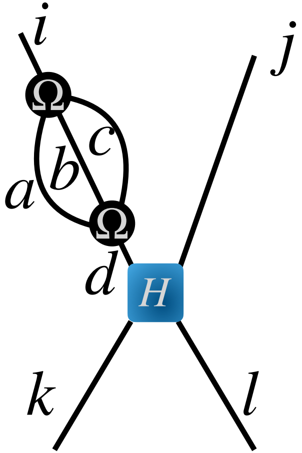



propagator
renormalization




vertex
renormalization

# *Why* does that topology dominate?




$$\frac{d}{ds}H_{ijkl} \sim \sum_{abcd} \Omega_{ciab}\Omega_{abcd}H_{djkl}$$

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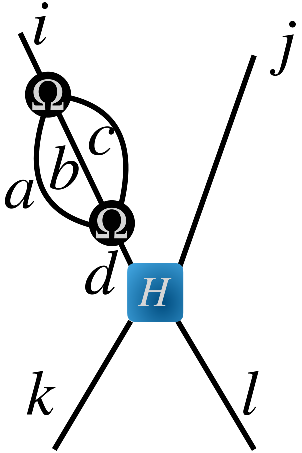


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for $i = d$ , this is $-|\Omega_{acbd}|^2$

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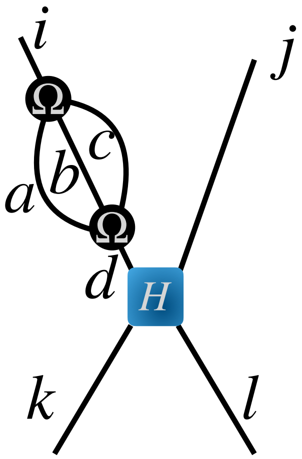


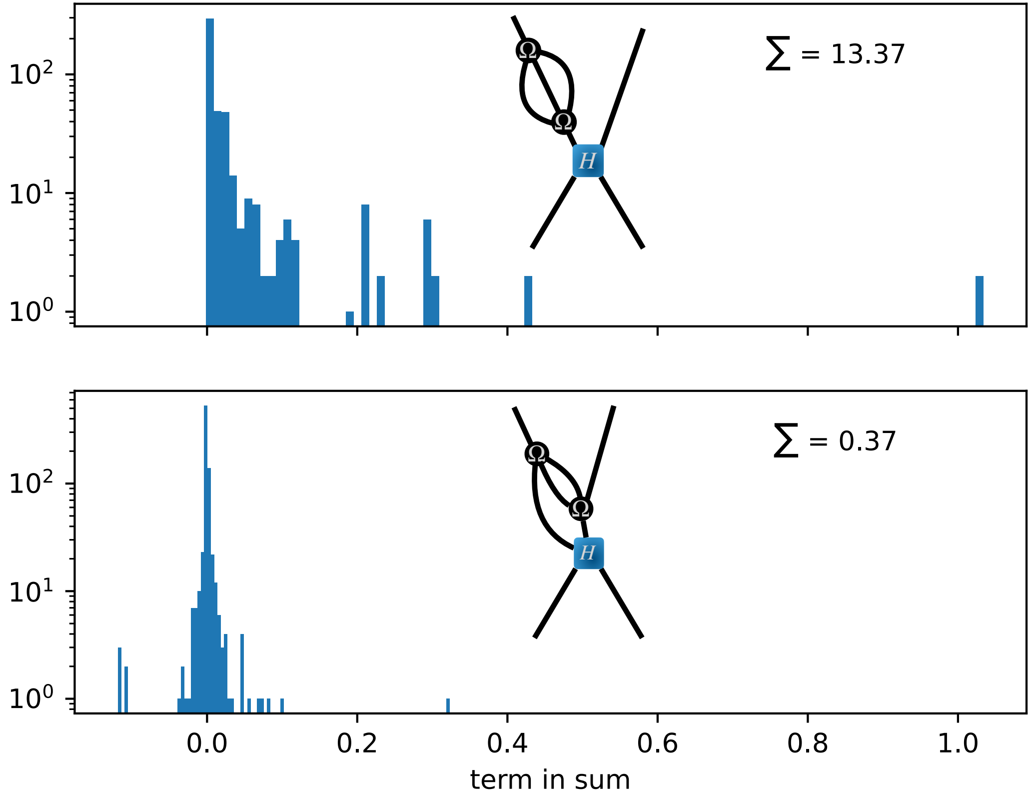

$$\frac{d}{ds}H_{ijkl} \sim \sum_{abcd} \underbrace{\Omega_{ciab}\Omega_{abcd}}H_{djkl}$$

for $i = d$ , this is $-|\Omega_{acbd}|^2$

$$\frac{d}{ds}H_{ijkl} \sim -H_{ijkl} \times \sum_{abcd} |\Omega_{acbd}|^2$$

all terms contribute with same sign!

# Histogram of individual terms in the sum



# Can we do even better? Probably.

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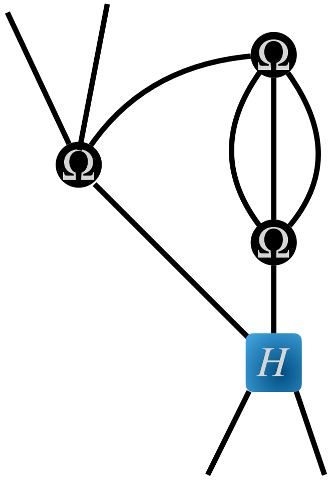
Next missing 1b,2b terms: $$\frac{1}{3!}\left[\Omega,\left[\Omega,[\Omega,H]_{3b}\right]_{3b,4b}\right]_{1b,2b}$$




IMSRG(4) diagram

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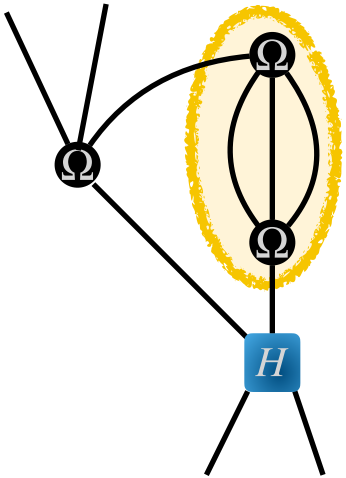


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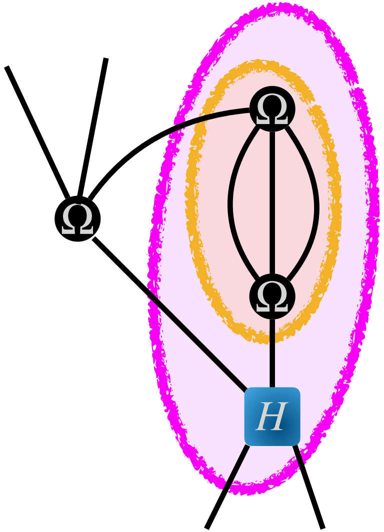


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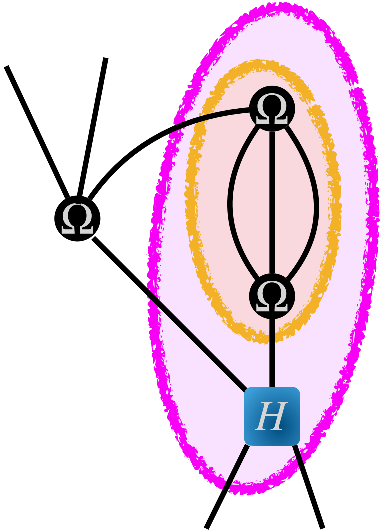


IMSRG(4) diagram

$$n^7 + n^9 + n^8 \longrightarrow n^5 + n^5 + n^6$$

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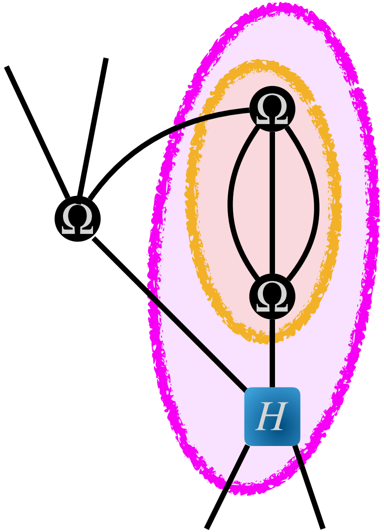


IMSRG(4) diagram

$$n^7 + n^9 + n^8 \longrightarrow n^5 + n^5 + n^6$$

or

$$\Delta H_{ijkl} \sim \sum_{abcdef} \Omega\Omega\Omega H \longrightarrow \text{Monte Carlo?}$$

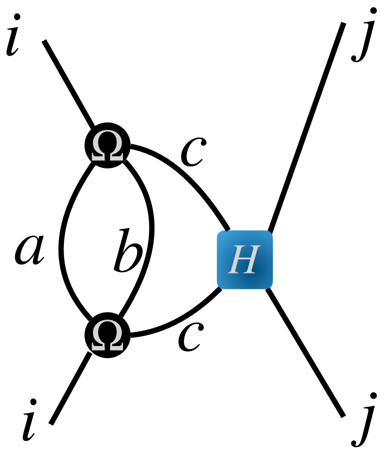
# Thank you!

This work also benefitted from conversations with many people, especially Matthias Heinz and Takayuki Miyagi.

Bingcheng He

Titus Morris

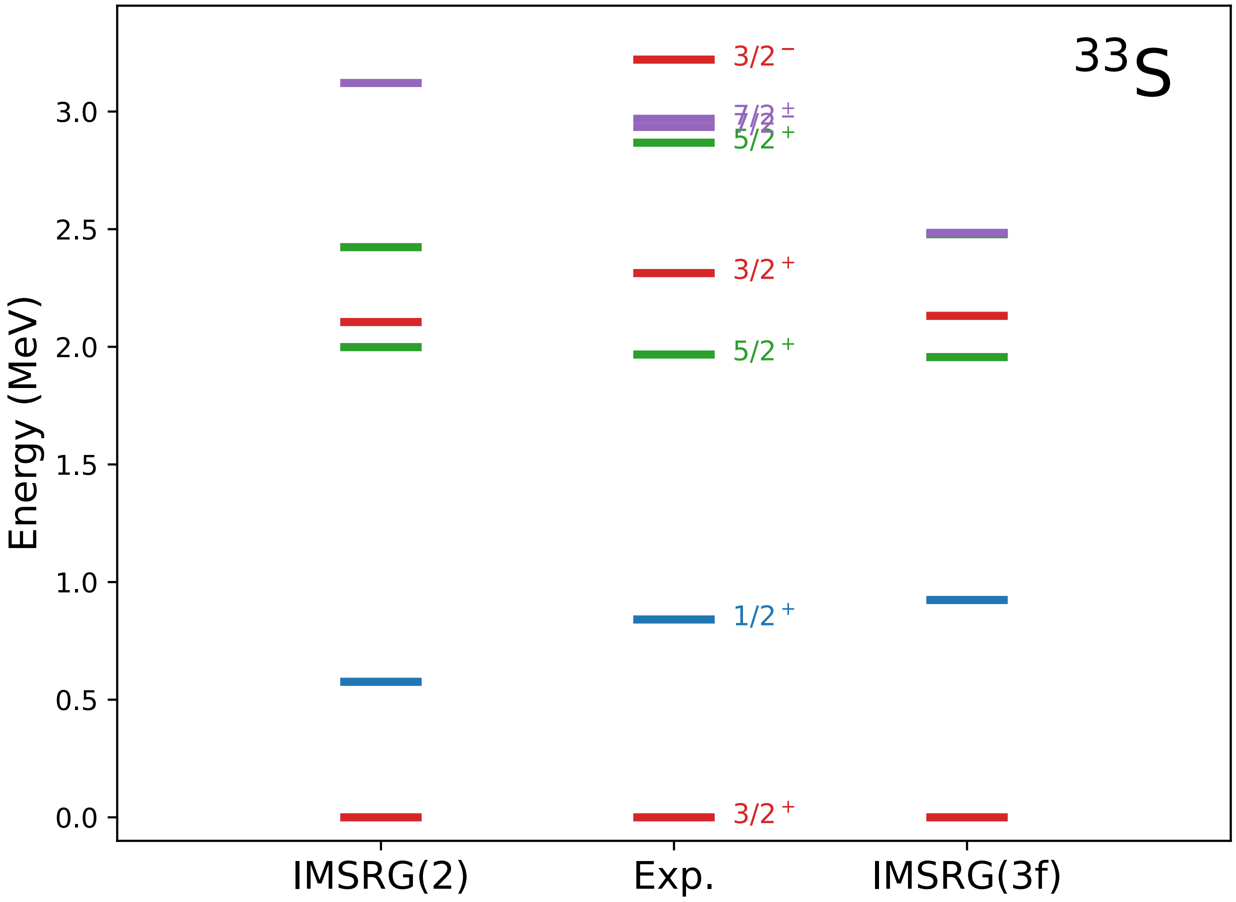
# Additional slides

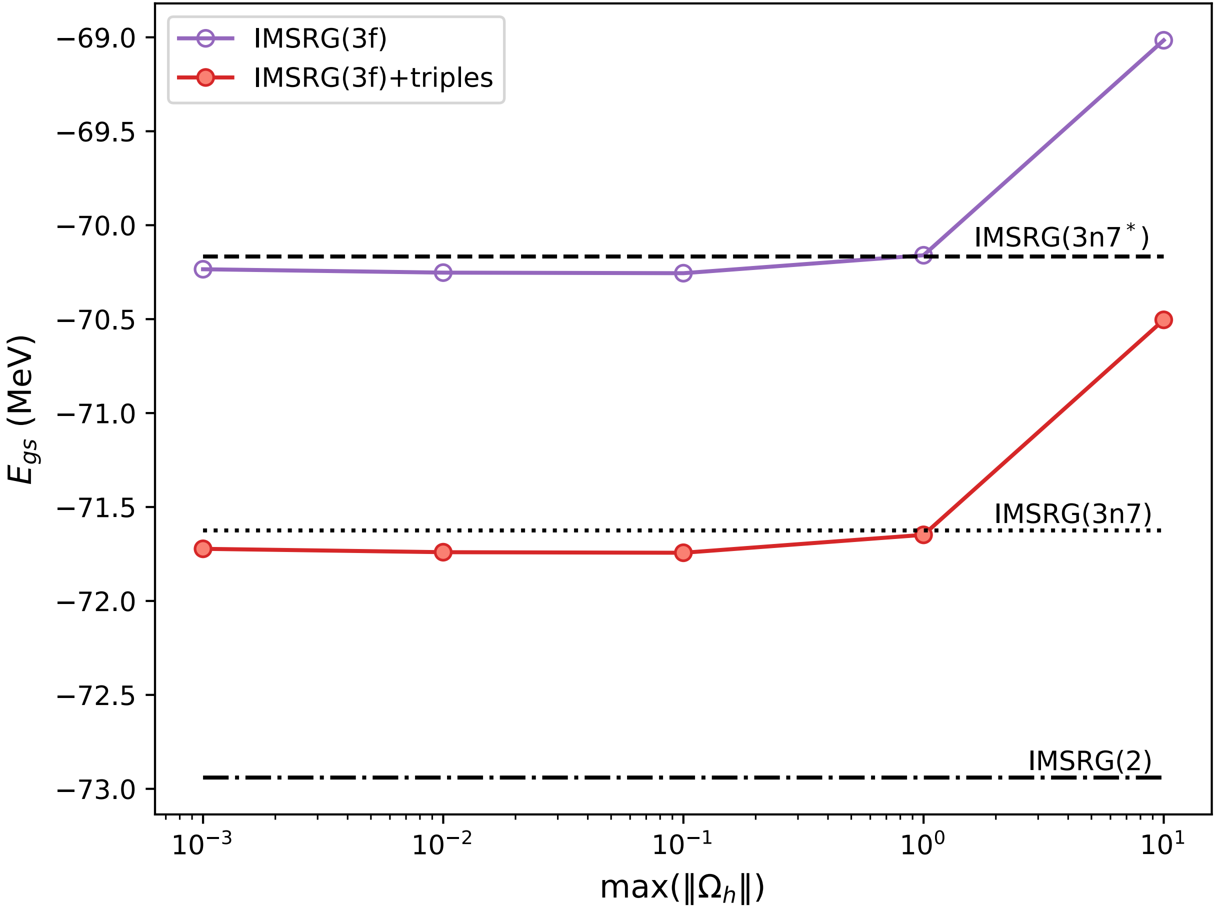



With random matrices, this is small, but for realistic H, the $H_{cjcj}$ tend to be negative.

$$\frac{d}{ds}H_{ijij} \sim \sum_{abc} \Omega_{iabj}\Omega_{bjia}H_{cjcj} \sim -\sum_{c} H_{cjcj} \times \sum_{ab} |\Omega_{iabj}|^2$$

# odd mass spectra



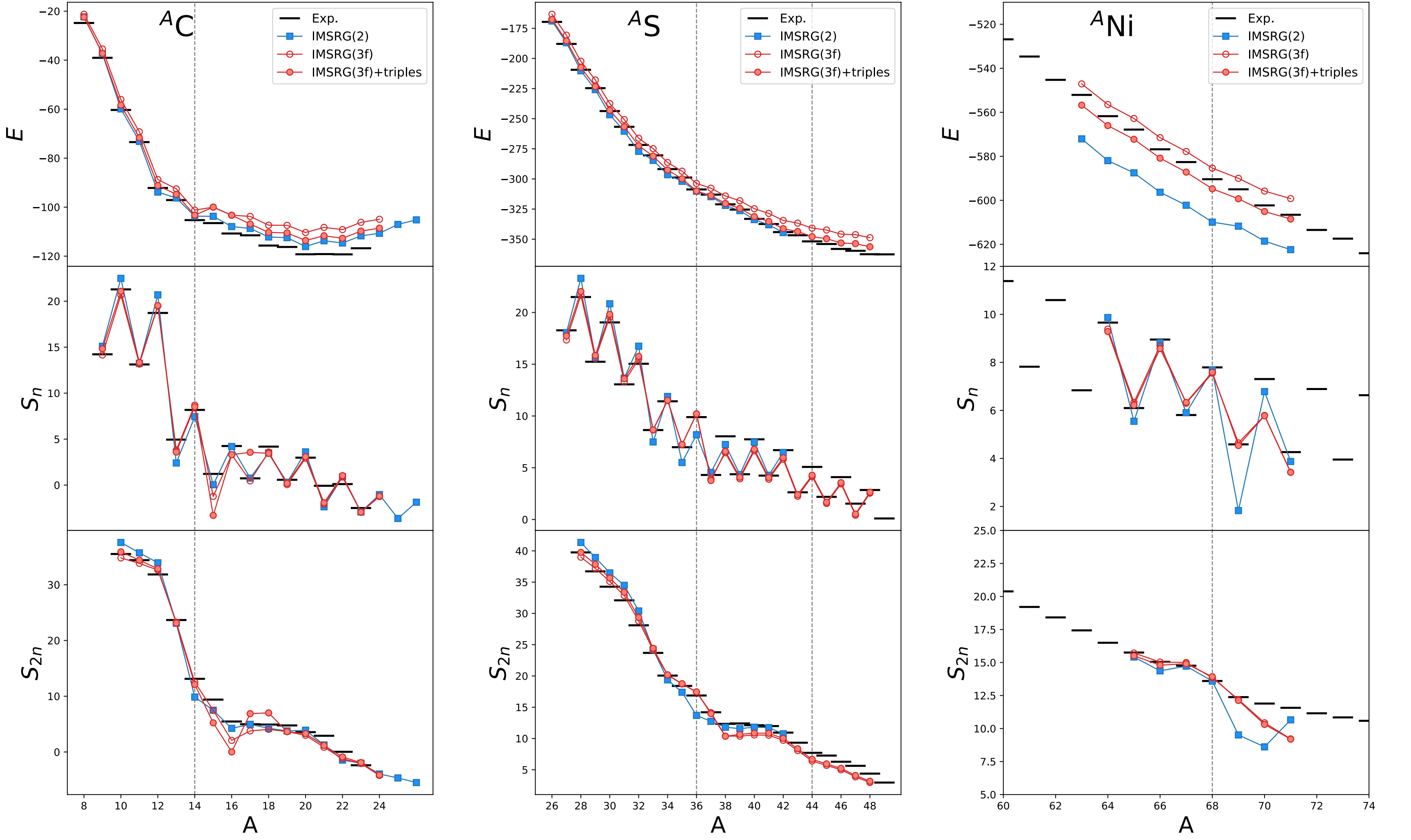



$$H(s) = UHU^\dagger$$

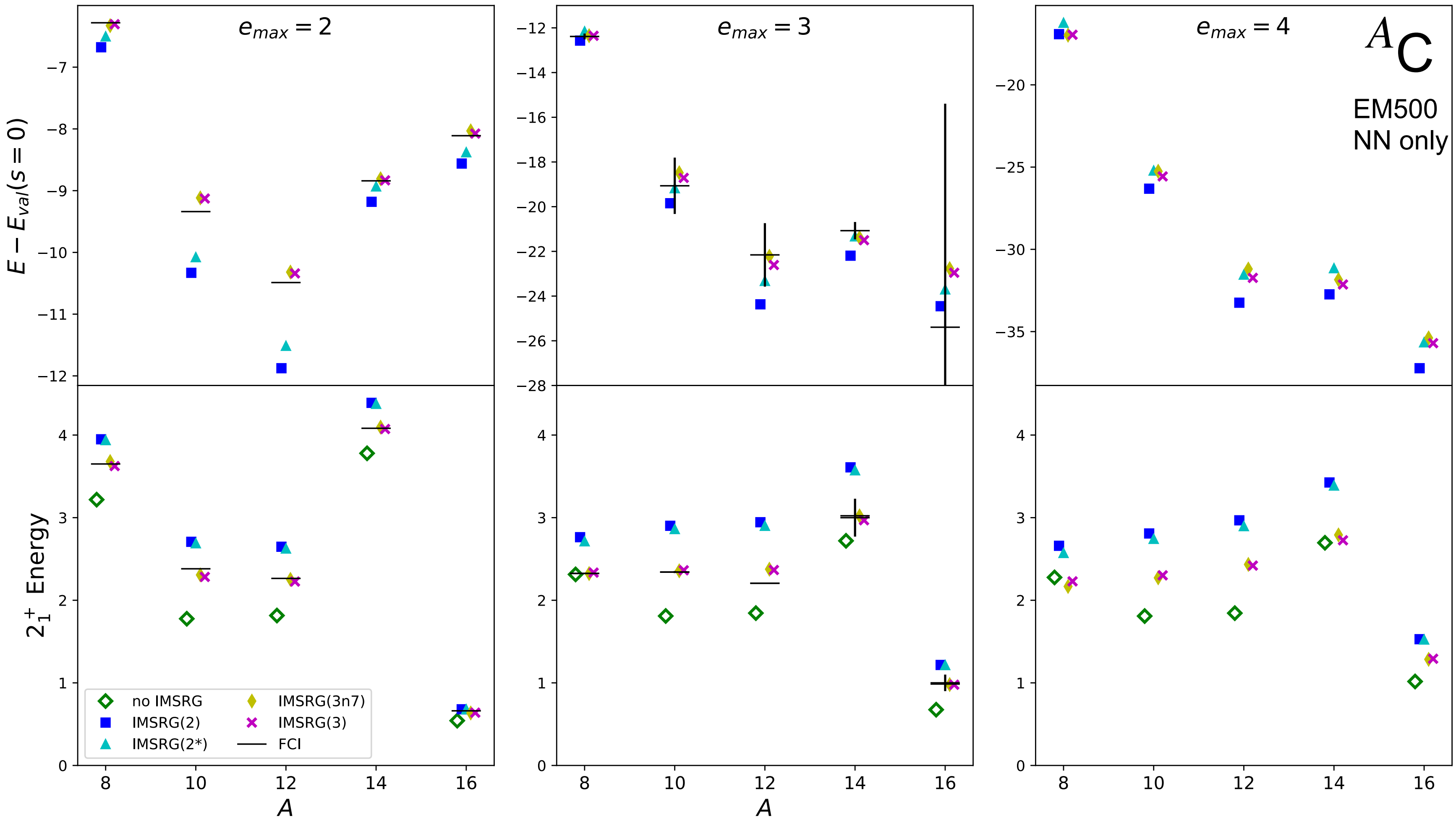
$$U = e^{\Omega_g} e^{\Omega_h}$$

gatherer

hunter



$^{A}$C
$^{A}$S
$^{A}$Ni
Exp.
IMSRG(2)
IMSRG(3f)
IMSRG(3f)+triples
E
$S_n$
$S_{2n}$
A



$e_{max} = 2$
$e_{max} = 3$
$e_{max} = 4$
$^A$C
EM500
NN only
$E - E_{val}(s=0)$
$2_1^+$ Energy
no IMSRG
IMSRG(2)
IMSRG(2*)
IMSRG(3n7)
IMSRG(3)
FCI
A