Analysis of three-body effects in the in-medium similarity renormalization group

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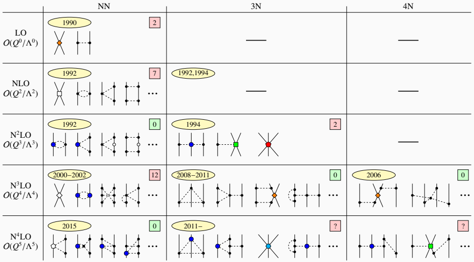
Ab initio nuclear structure

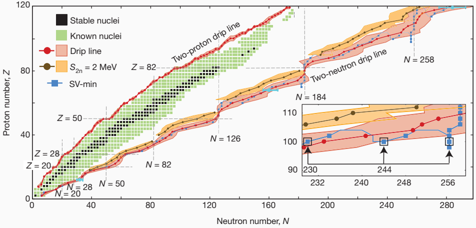
Ab initio approach:

1. Determine nuclear interactions
2. Solve many-body problem
3. (1) & (2) should be systematically improvable

Benefits:

- Physics insights
- Predictive power
- Quantify uncertainties

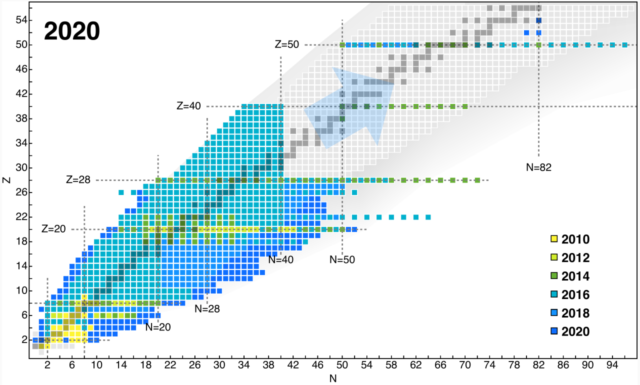




Top: Hebeler, 2020, Bottom: Erler *et al.*, Nature **486**, 2012

Recent ab initio progress

- 2010: mostly results in range of exact methods (NCSM, QMC)
- 2010-2015: many-body expansion methods able to target (near) closed-shell nuclei
- 2015-2020: full *ab initio* description of mid-mass open- and closed-shell systems

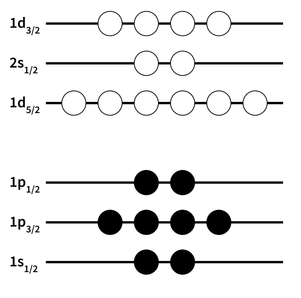


Hergert, Front. Phys. **8**, 2020

Essence of many-body expansion methods

Examples: CI, MBPT, CC, SCGF, IMSRG

$$|\Psi\rangle \approx |\Phi\rangle$$



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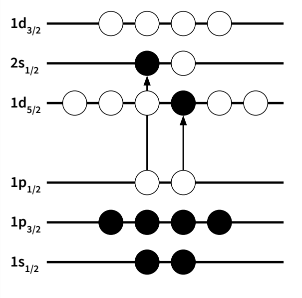

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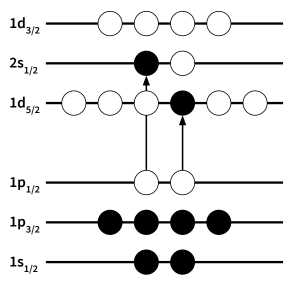

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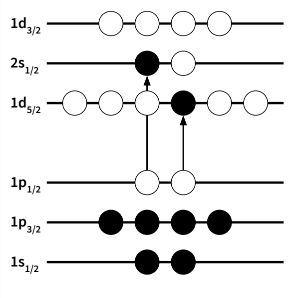

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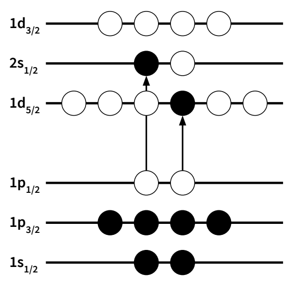


$|\Phi_{ij}^{ab}\rangle$

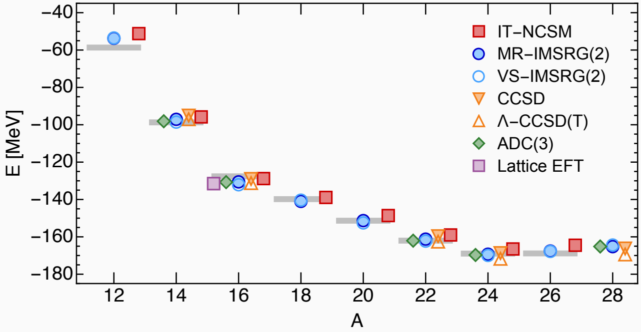
IMSRG formalism gives rise to IMSRG(2) and IMSRG(3) truncations

IMSRG(3) in the many-body context

Many-body expansion is "under control"

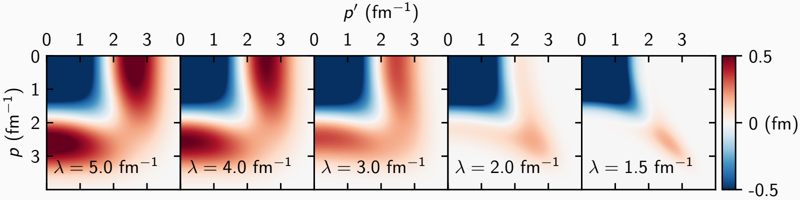
Why go to IMSRG(3)?

- Confirm many-body expansion behavior
- Higher precision in light and medium-mass nuclei
- UQ for many-body expansion
- Approximate IMSRG(3) for heavy nuclei
- Study behavior for other observables



Hergert, Front. Phys. **8**, 2020

Similarity renormalization group Bogner, Furnstahl, Perry, PRC **75**, 2007



Continuous unitary transformation:

$$H(s) = U(s)H(s=0)U^\dagger(s)\,, \qquad \frac{dH(s)}{ds} = [\eta(s), H(s)]$$

The SRG evolution...

- decouples low- and high-energy states,
- but induces many-body forces.

In-medium similarity renormalization group (IMSRG) Tsukiyama, Bogner, Schwenk, PRL **106**, 2011

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IMSRG(2):

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NO2B approximation:

- Approximate treatment of initial three-body force
- $\bar{H}^{(2)}_{pqrs} = H^{(2)}_{pqrs} + \sum_i H^{(3)}_{pqirsi}$

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IMSRG(3):

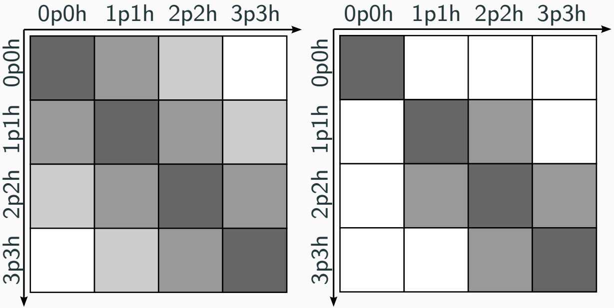
$$H(s) \approx \bar{H}^{(0)}(s) + \bar{H}^{(1)}(s) + \bar{H}^{(2)}(s) + \bar{H}^{(3)}(s)$$
$$\eta(s) \approx \eta^{(1)}(s) + \eta^{(2)}(s) + \eta^{(3)}(s)$$

Normal ordering:

- Complete inclusion of initial normal-ordered Hamiltonian
- Approximate evolution of many-body forces (both IMSRG(2) and IMSRG(3))

Decoupling in the IMSRG in closed-shell systems

- Decouple $|\Phi\rangle$ from its excitations
- $E(s \to \infty) = \langle \Phi | H(s \to \infty) | \Phi \rangle$ is the energy of the targeted state
- Observe: MBPT corrections vanish for $s \to \infty$



$\langle i | H(s=0) | j \rangle$ $\langle i | H(s \to \infty) | j \rangle$

Hergert *et al.*, Phys. Rept. **621**, 2016

Fundamental commutators

“Fundamental”: commutators are the basic computational operation

$$\left[A^{(K)}, B^{(L)}\right] = \sum_{M=|K-L|}^{K+L-1} C^{(M)}$$

Schematic notation:

$$[K, L] \to M$$

w/ computational cost $\mathcal{O}(N^{K+L+M})$ where N is the size of the computational basis

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IMSRG(3) commutators:

$$\begin{aligned}
\mathcal{O}(N^6): &\quad [1,3] \to 2\,, [2,3] \to 1\,, [3,3] \to 0 \\
\mathcal{O}(N^7): &\quad [2,2] \to 3\,, [1,3] \to 3\,, [2,3] \to 2\,, \\
&\quad [3,3] \to 1 \\
\mathcal{O}(N^8): &\quad [2,3] \to 3\,, [3,3] \to 2 \\
\mathcal{O}(N^9): &\quad [3,3] \to 3
\end{aligned}$$

- $[2,2] \to 3$ induces neglected three-body part in IMSRG(2)
- $[3,3] \to 3$ is most expensive
- Note: Λ-CCSD(T) is $\mathcal{O}(N^7)$

IMSRG(3) computational challenges

O_{pqrstu}:

- Rank-6 tensor with $\mathcal{O}(N^6)$ storage cost
- ~ 30 GB at $e_{\max} = 2$

$\sum_{abc} \eta^{(3)}_{ijkabc} \bar{H}^{(3)}_{abclmn}$:

- Huge matrix-matrix multiply
- $\mathcal{O}(10^{14})$ FLOPs at $e_{\max} = 2$

Challenging at $e_{\max} = 2$
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Exploitable symmetries:

- Isospin conservation
- Parity conservation
- **Rotational invariance**

Angular-momentum coupling for the IMSRG

- Express everything in terms of eigenstates of J_z and J^2
- Analytically simplify angular-momentum projection dependence
- Go from states $|p\rangle = |\tilde{p} m_p\rangle$ to “reduced” orbitals $\tilde{p}$

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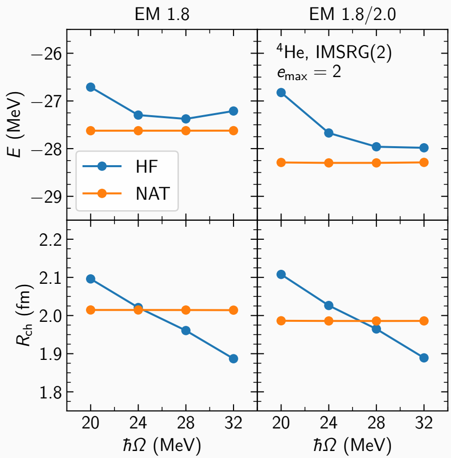
	Basis	Uncoupled MEs	Coupled MEs
One-body	$\lvert\tilde{p} m_p\rangle$	O_{pq}	$O^{j_p}_{\tilde{p}\tilde{q}}$
Two-body	$\lvert(\tilde{p}\tilde{q}) J_{pq} M_{pq}\rangle$	O_{pqrs}	$O^{J_{pq}}_{\tilde{p}\tilde{q}\tilde{r}\tilde{s}}$
Three-body	$\lvert[(\tilde{p}\tilde{q}) J_{pq} \tilde{r}] J_{pqr} M_{pqr}\rangle$	O_{pqrstu}	$O^{(J_{pqr}, J_{pq}, J_{rs})}_{\tilde{p}\tilde{q}\tilde{r}\tilde{s}\tilde{t}\tilde{u}}$

Automatic angular-momentum coupling of fundamental commutators performed using `amc` program (Tichai *et al.*, 2020)

^{4}He in IMSRG(2) Hamiltonian details



$$H_{\text{int}} = T_{\text{int}} + V^{(2)}(+V^{(3)})$$

NN-only case:

- N^{3}LO EM potential with $\Lambda = 450\,\text{MeV}$ SRG-evolved to $\lambda = 1.8\,\text{fm}^{-1}$
- "EM 1.8"

NN+3N case (**NO2B**):

- 3N potential fit after SRG evolution to reproduce $E_{^3\text{H}}$ and $R_{^4\text{He}}$
- "EM 1.8/2.0"

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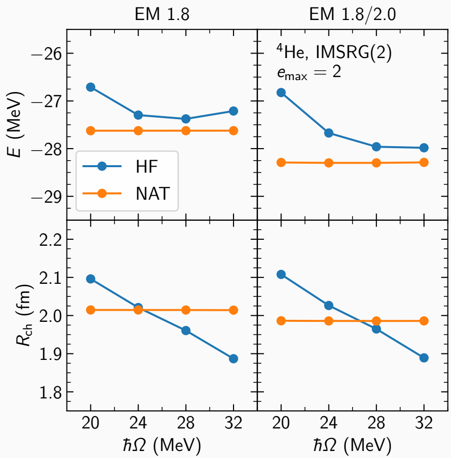

$e = 2n + l \leq e_{max} = 2$ model space:

- 12 reduced orbitals $\tilde{p}$
- 6 two-body channels
- 132 three-body channels

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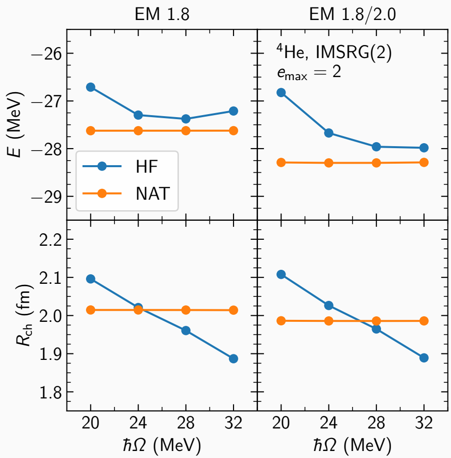

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Hartree-Fock (HF) basis:

- Constructed in $e_{\text{max}} = 2$

Natural orbitals (NAT) basis: (Hoppe *et al.*, 2020)

- Eigenbasis of perturbatively-constructed density
- Constructed in $e_{\text{max}} = 14$ ($E_{3\text{max}} = 16$)

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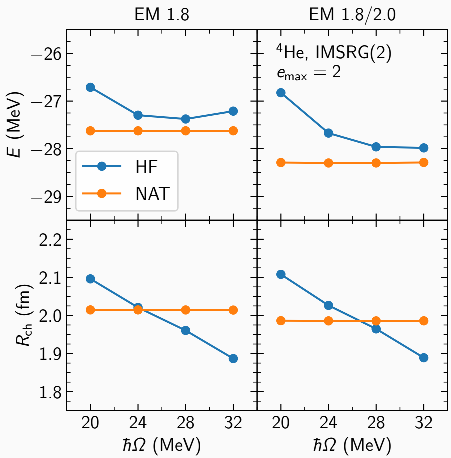

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- Cannot compare to experiment
- Ideal comparison would be to $e_{max} = 2$ CI

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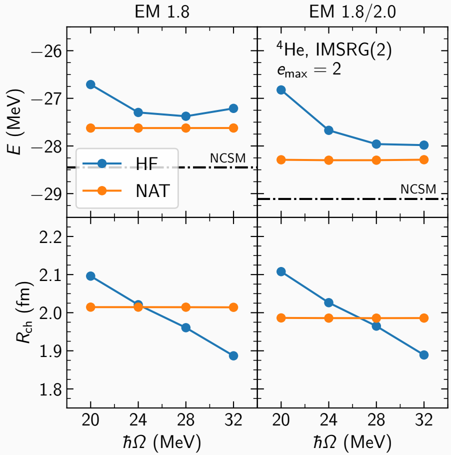

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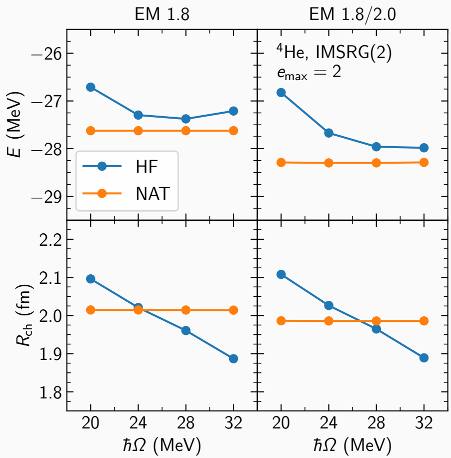

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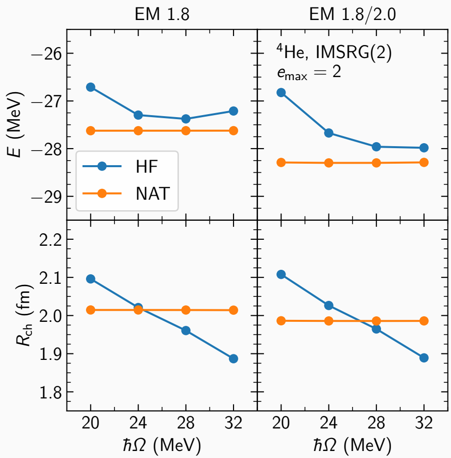

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Trends:

- Inclusion of 3N forces gives slightly more binding energy and a slightly smaller charge radius
- NAT results are independent of $\hbar\Omega$

Approximate IMSRG(3) truncation schemes

Idea:

- Start with IMSRG(2)
- Selectively add IMSRG(3) commutators
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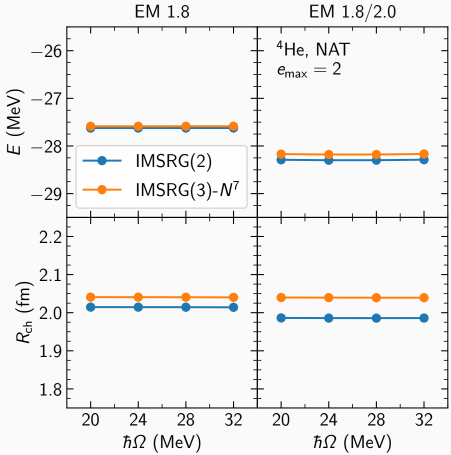
^{4}He in IMSRG(3)-N^7



- Small effect on energies
  - $\sim$ 40 keV for NN-only
  - $\sim$ 100 keV for NN+3N
- Larger effect on radii
  - $\sim$ 0.025 fm for NN-only
  - $\sim$ 0.054 fm for NN+3N
  - Still in few percent range

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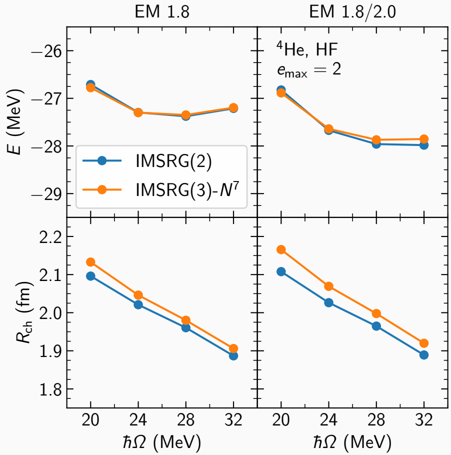
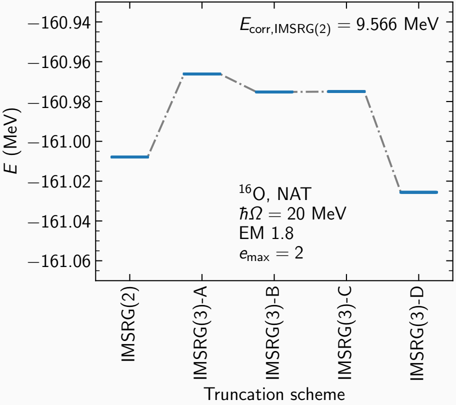


- Same trends as NAT basis
- Freqency dependence seems slightly flatter in energies
- No similar behavior for radii
- Will be interesting to look at trends in larger model spaces

Truncation scheme investigation in ^{16}O



- Overall, all corrections are small (sub-100 keV for 160 MeV binding energy)
- IMSRG(3)-A produces a relatively large shift
- IMSRG(3)-B (with $\mathcal{O}(N^6)$ commutators) and IMSRG(3)-C produce very small shifts
- IMSRG(3)-D (first $\mathcal{O}(N^8)$ commutator) produces the largest shift

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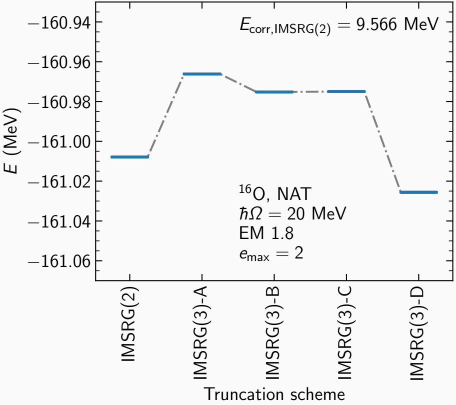

$$\begin{aligned}
\text{IMSRG(3)-A} &= \text{IMSRG(2)} + \color{red}{[2,2] \to 3} \\
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- IMSRG(3)-N^7 gives corrections on the order of per mille for energies and few percent for radii
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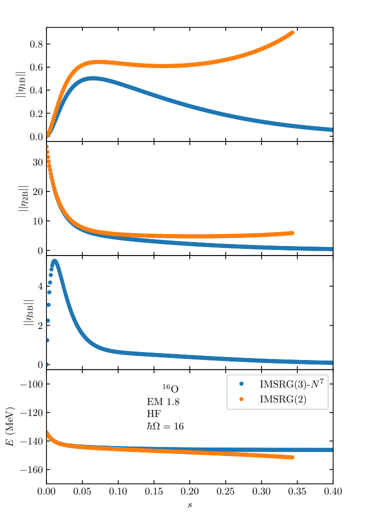
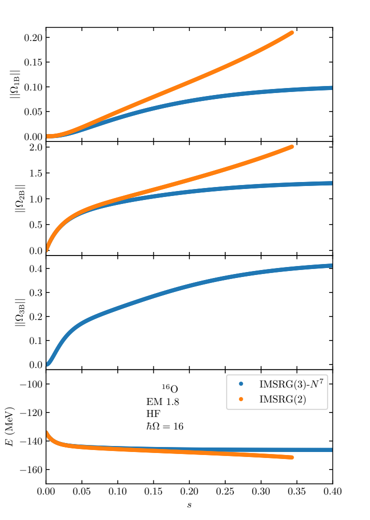
Thank you for your attention!

Flow in ^{16}O - HF





Flow in ^{4}He - HF