Approximations and uncertainties in the in-medium similarity renormalization group

Matthias Heinz *with Jan Hoppe, Alexander Tichai, Kai Hebeler, and Achim Schwenk*

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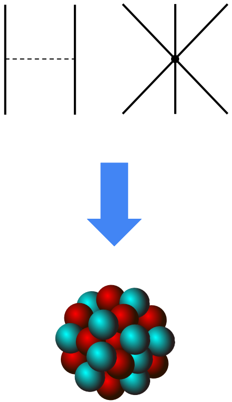
Ab initio many-body theory



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

Goal: Describe many-body system using only few-body interactions as input

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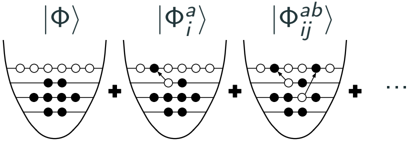

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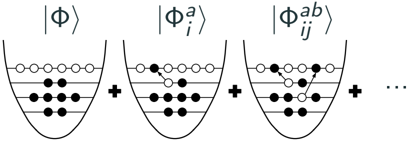

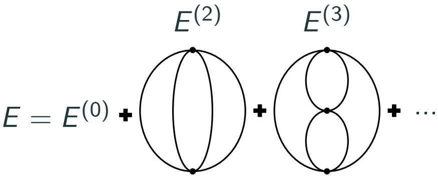

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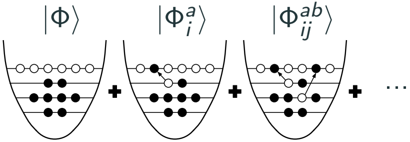

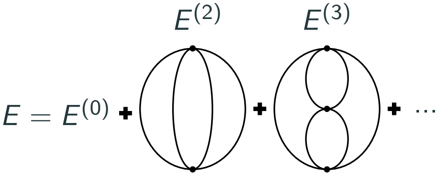

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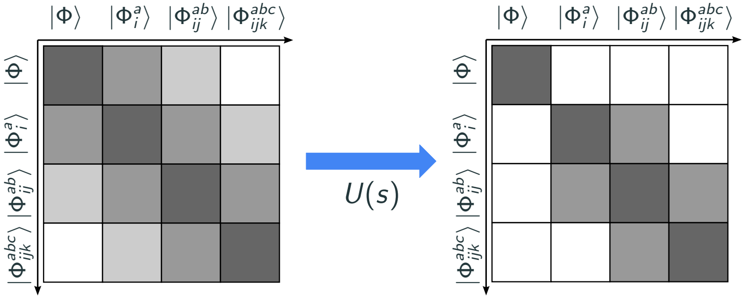
- What is error due to many-body truncation?

The in-medium similarity renormalization group

Tsukiyama, Bogner, Schwenk, PRL **106** (2011)



initial H diagonalized H

Hergert *et al.*, Phys. Rep. **621** (2016)

SRG flow equation:

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

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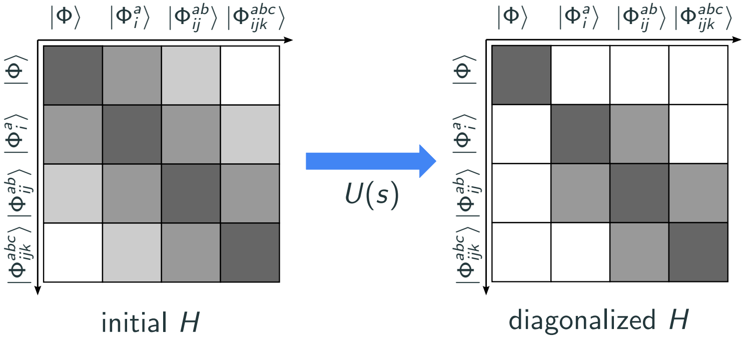

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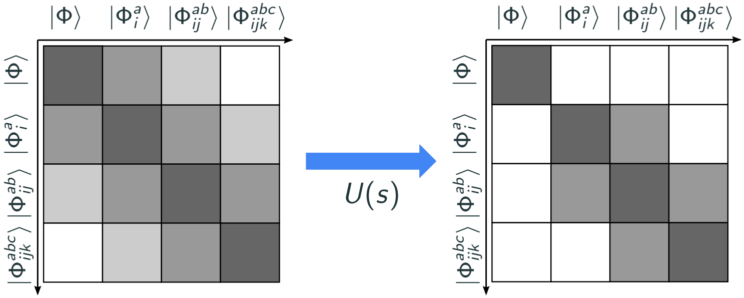

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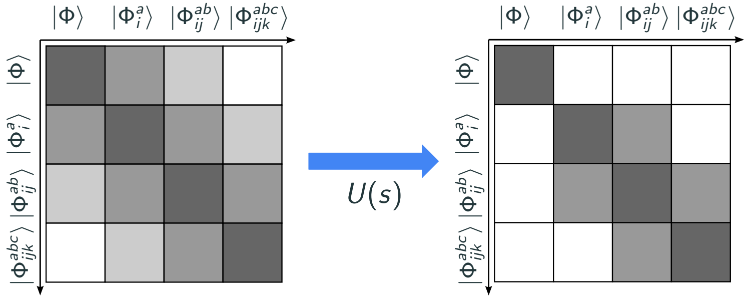

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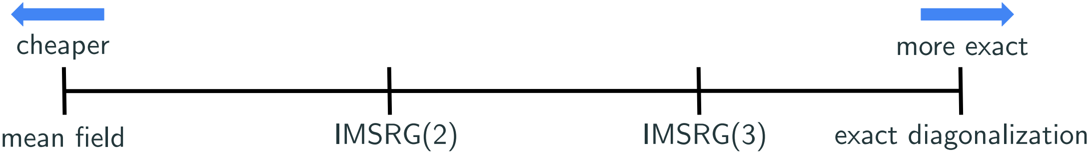
Investigating the many-body expansion

MH, Tichai, Hoppe, Hebeler, Schwenk, PRC **103** (2021)



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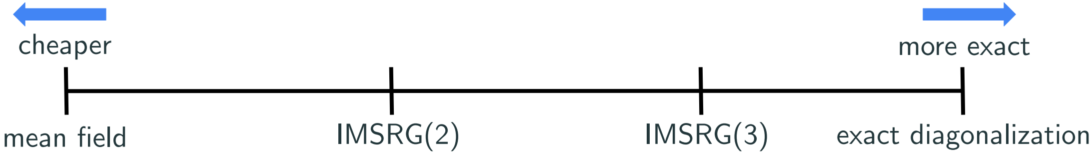

- Systematic expansion to approximate exact result
- Ideal study: compare IMSRG(2) and IMSRG(3) to exact results
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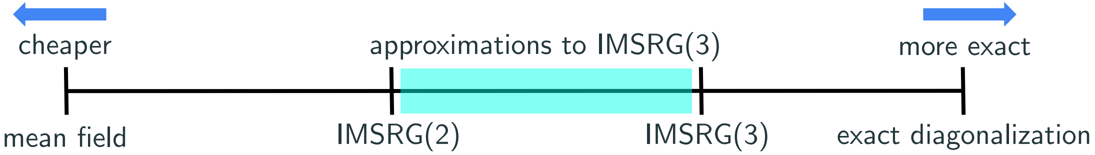

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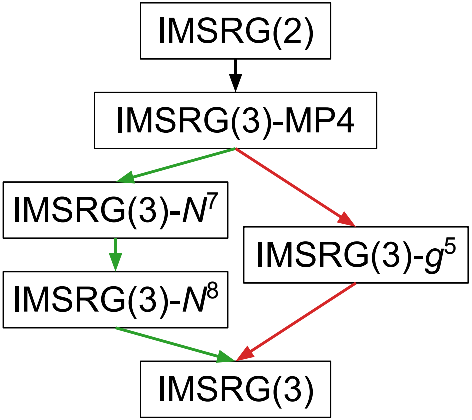
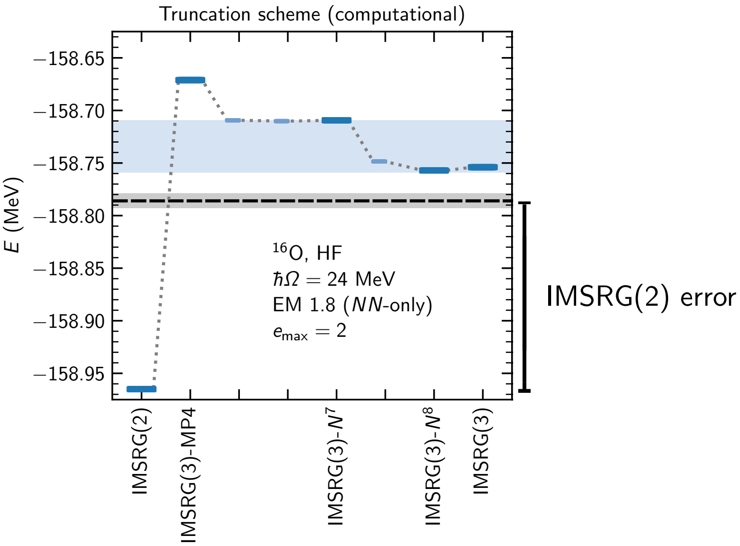
- Ideal study: compare IMSRG(2) and IMSRG(3) to exact results
  - Only possible in small systems
- Study truncations that approximate IMSRG(3) at lower computational cost

Going from IMSRG(2) to IMSRG(3)

- 10 new terms in IMSRG(3)
- 4 included in IMSRG(3)-MP4 (minimal extension of IMSRG(2))
- Remaining terms can be categorized according to:
  - Computational cost ($\mathcal{O}(N^7)$ - $\mathcal{O}(N^9)$)
    - $\mathcal{O}(N^7) \sim$ 8 minutes
    - $\mathcal{O}(N^9) \sim$ 14 hours
  - Perturbative importance (g^5, g^6)
    - MP4 contains all g^4 terms



Application in oxygen-16



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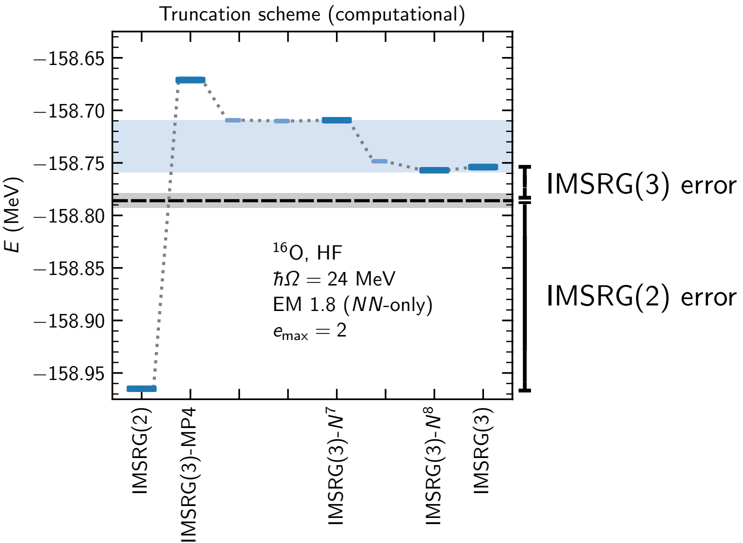

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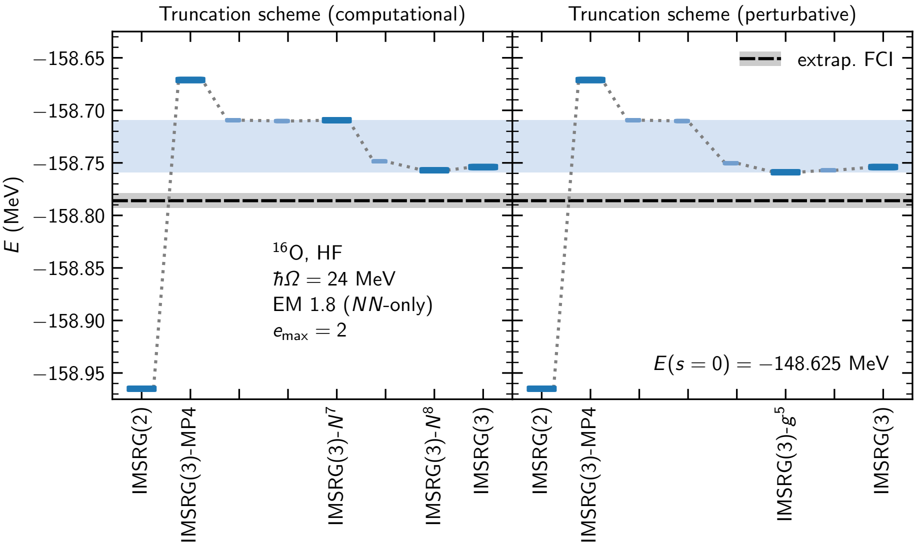

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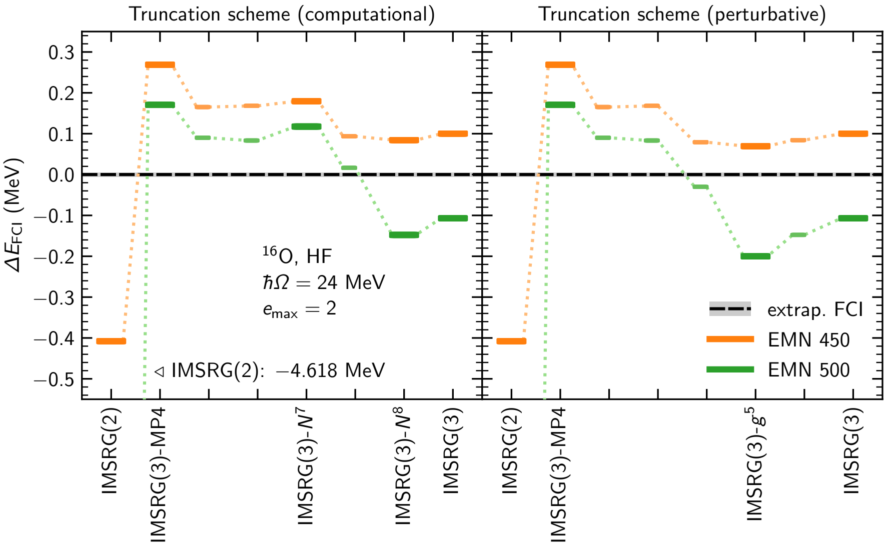
Results for other Hamiltonians



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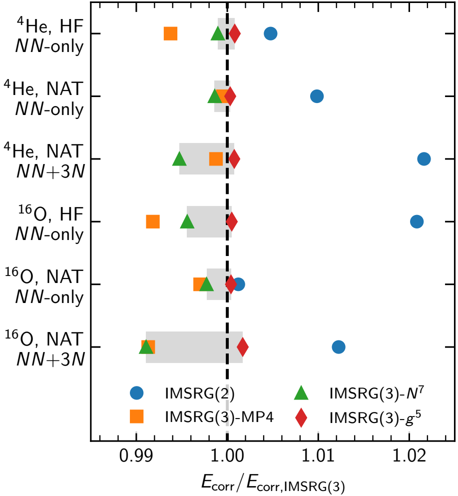
General trends for approximating the IMSRG(3)



- IMSRG(3) well approximated by:
  - IMSRG(3)-N^7 (lower cost)
  - IMSRG(3)-g^5 (higher cost)
- Use 2 different truncations to estimate IMSRG(3) approximation error:
  - Easy: IMSRG(2) and IMSRG(3)-MP4
  - Better: IMSRG(3)-N^7 and IMSRG(3)-g^5

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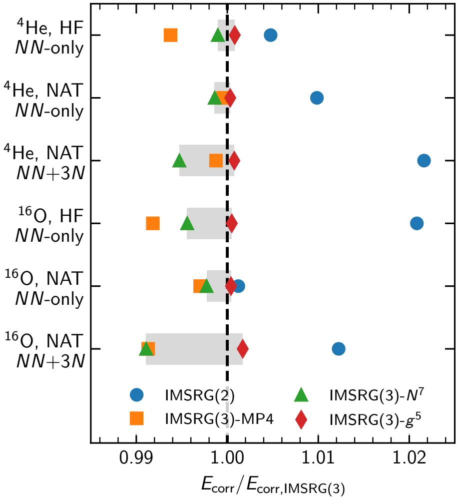

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  - Easy: IMSRG(2) and IMSRG(3)-MP4
  - Better: IMSRG(3)-N^7 and IMSRG(3)-g^5
- IMSRG(3) approximation error is a *proxy* for many-body error

MH, Tichai, Hoppe, Hebeler, Schwenk, PRC **103** (2021)

Outlook

Key takeaways:

- IMSRG many-body expansion converges systematically
- IMSRG(3) convergence benefits can be approximated at lower computational cost
- Many-body UQ is possible!

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Next developments:

- Apply (approximate) IMSRG(3) to large-scale calculations of nuclei . . .
- . . . including other observables
- Accelerate IMSRG calculations to enable more expensive truncations:
  - Improved basis construction
  - Importance truncation to discard unimportant (three-body) matrix elements

Hoppe *et al.*, PRC **103** (2021)

Hoppe *et al.*, arxiv:2110.09390 (2021)

- Refine UQ for many-body calculations (emulators, model mixing, etc.)

Discussion points and acknowledgments

- How can we best leverage our sequentially refined models using Bayesian tools?
- What features of (extremely expensive) many-body calculations can be leveraged to develop improved emulators?

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Thank you to my collaborators:

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- Achim Schwenk,
- and more at the TU Darmstadt and beyond.

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Thank you for your attention!