TECHNISCHE UNIVERSITÄT DARMSTADT

FLEXIBLE IMSRG EVOLUTION FOR ACTIVE SPACE HAMILTONIANS

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MITP – Many-Body Theory: Nuclear Physics Meets Quantum Chemistry, Mainz, Germany

LOEWE
Exzellente Forschung für Hessens Zukunft

OUTLINE

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INTRODUCTION TO IMSRG

- Idea of IMSRG *(see also: talks by H. Hergert, T. Miyagi and M. Cincar)*
- Generator choice

FLEXIBLE IMSRG ACTIVE SPACE HAMILTONIANS

- Idea
- Workflow
- Preliminary results

OUTLOOK & CONCLUSION

IN-MEDIUM SIMILARITY RENORMALIZATION GROUP (IMSRG)

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K. Tsukiyama, S.K. Bogner and A. Schwenk, Phys. Rev. C **85,** 061304(R) (2012)
H. Hergert, et al. Phys Rept. **621** 165-222 (2016)

- Diagonalize the Hamiltonian via a continuous unitary transformation with flow parameter s

$$H(s) = U(s)H(0)U^\dagger(s)$$

- Flow equation:

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

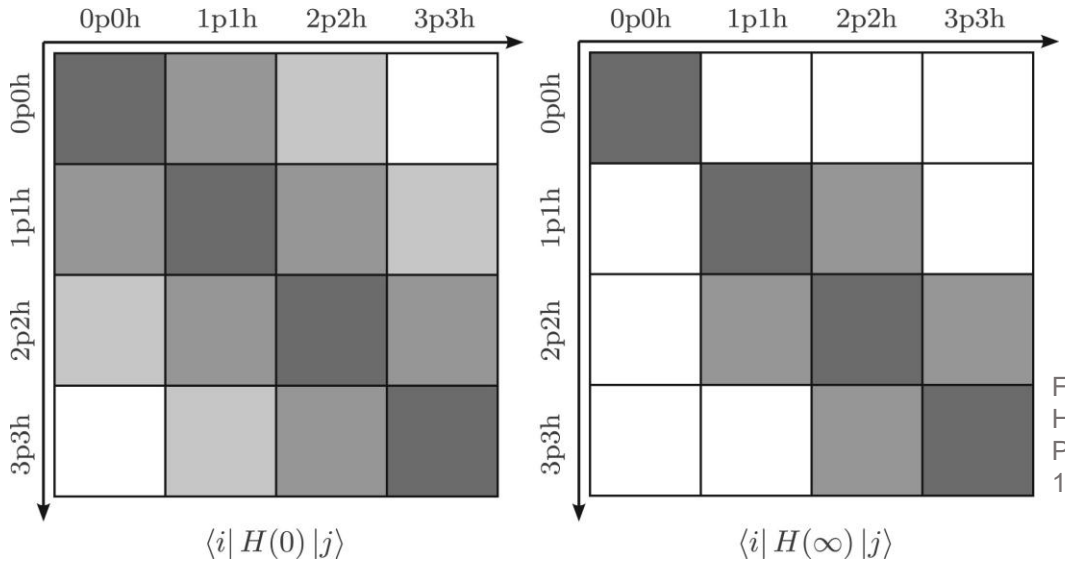

Figure from: H. Hergert, et al. Phys Rept. **621**, 165-222 (2016)

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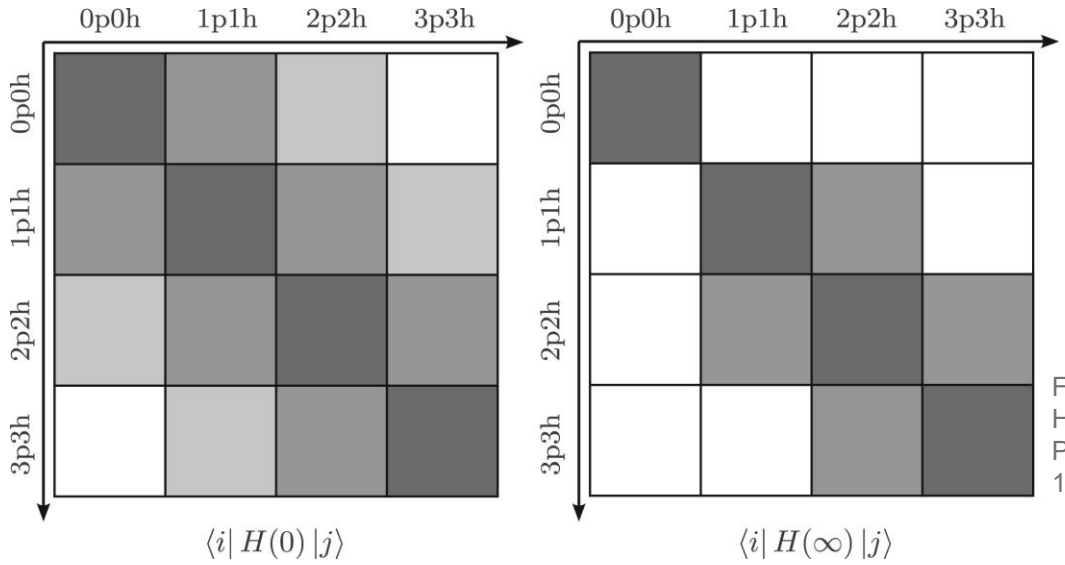


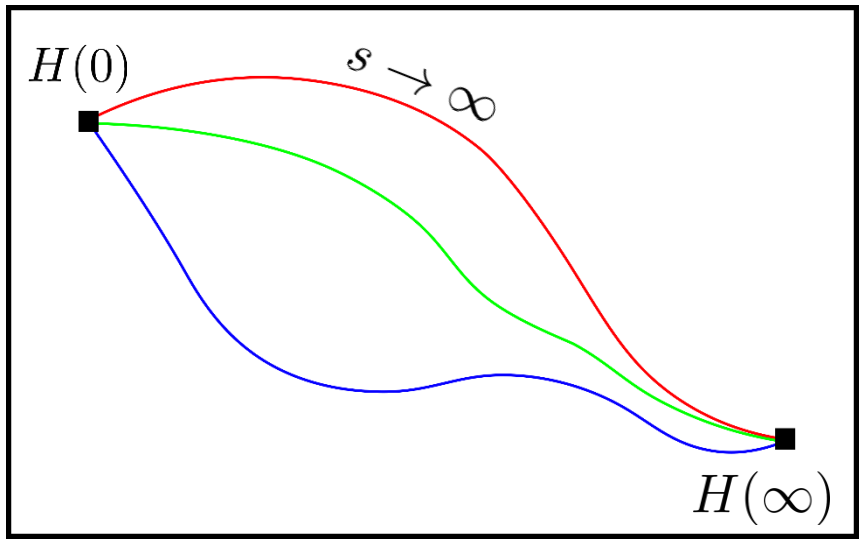
Figure from: H. Hergert, et al. Phys Rept. **621**, 165-222 (2016)

GENERATOR CHOICE

- Information about the flow is captured through the generator η

$$\eta \sim f(H_{\mathrm{od}})$$

- f dictates the shape of the flow
- $H_{\mathrm{od}} = H - H_{\mathrm{d}}$ is part of Hamiltonian that is being decoupled and defines the stationary point of the flow
- s is the distance along the flow



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Aims:

- Use of arbitrary reference states
- Decoupling of arbitrary spaces from the rest of the model space
- Retaining more information after evolution
- Reducing model space sizes for post-processing methods
- …

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VS-IMSRG:
S.K. Bogner, et al. Phys. Rev. Lett., **113** 0142501 (2014)
S.R. Stroberg, et.al. Phys. Rev. Lett., **118** 032502 (2017)
T. Miyagi, et al. Phys. Rev. C, **102** 034320 (2020)
Active space:
Work by C. Wenz and R. Roth

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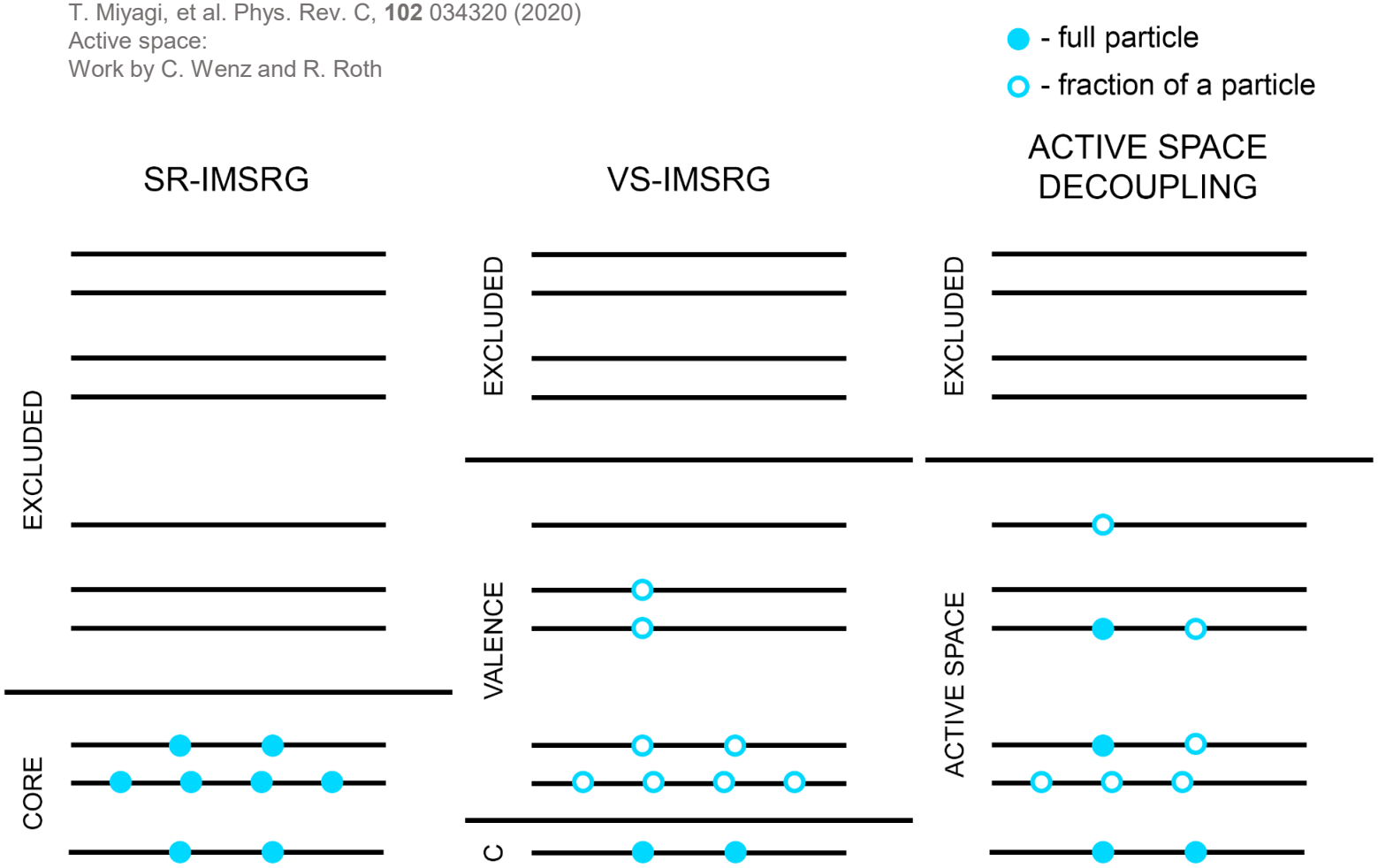
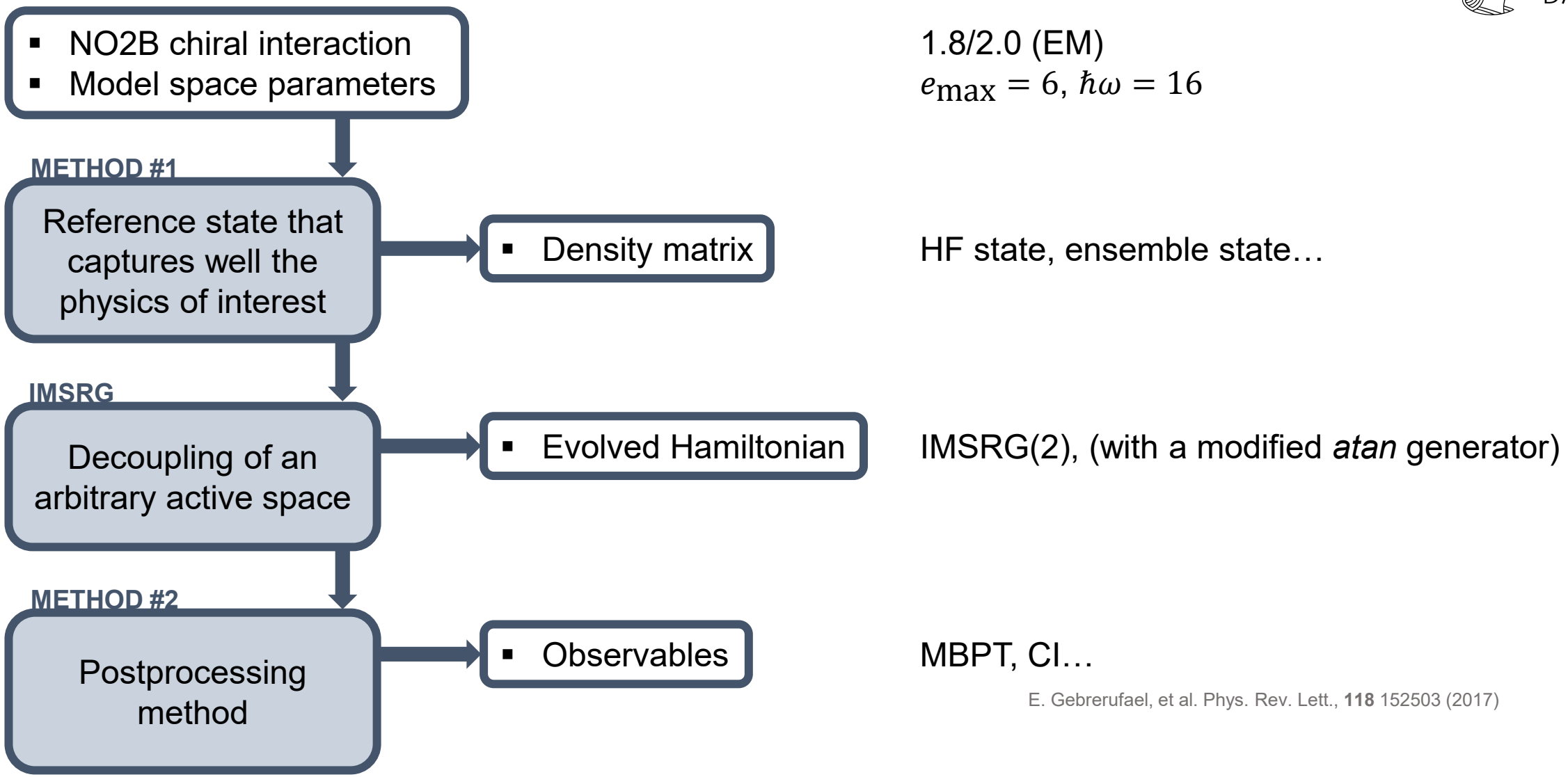
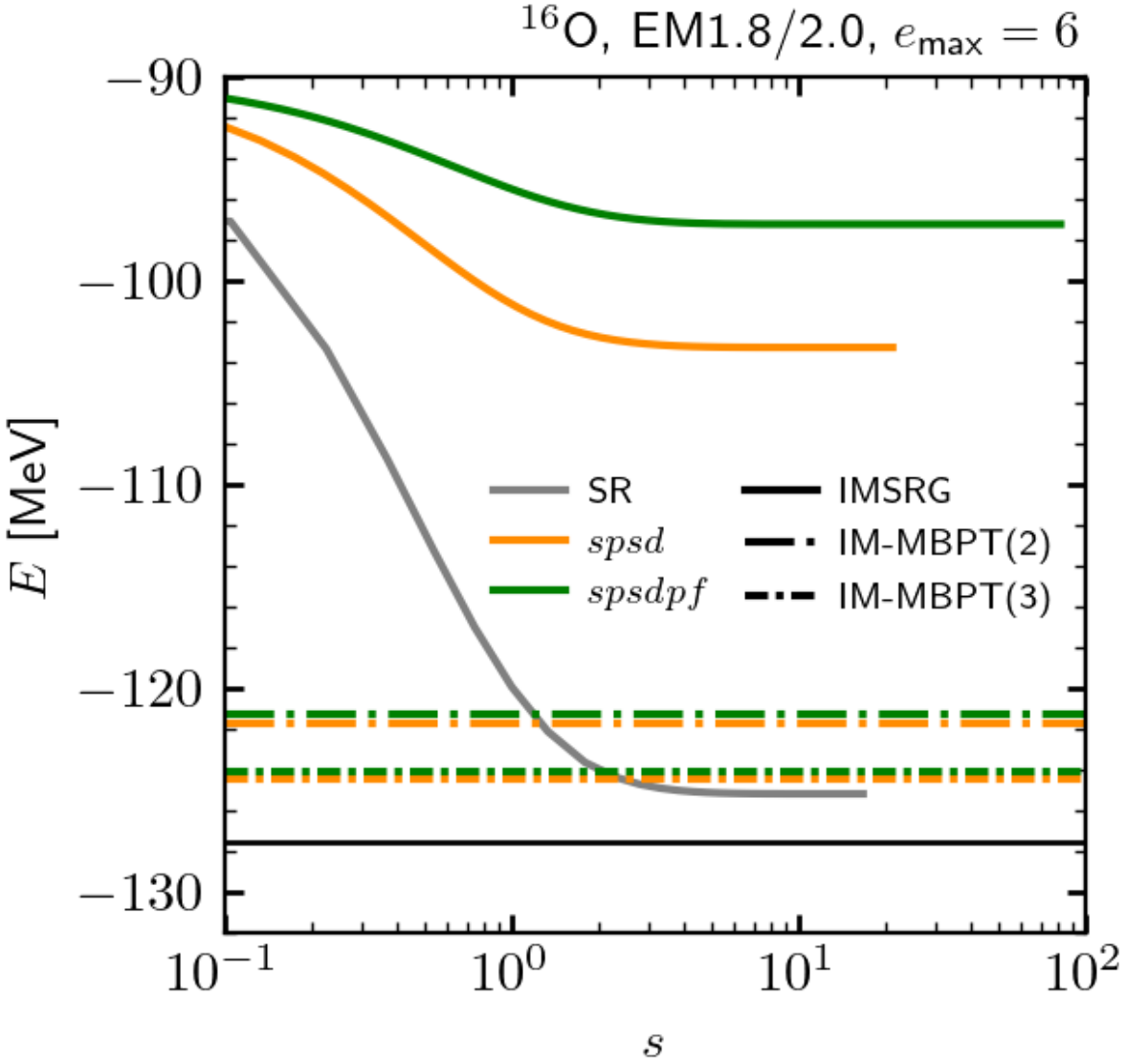


WORKFLOW



E. Gebrerufael, et al. Phys. Rev. Lett., **118** 152503 (2017)

PRELIMINARY RESULTS



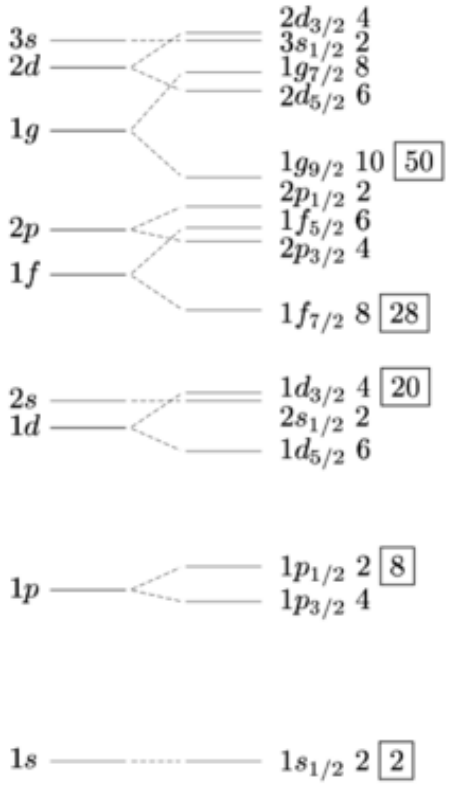


Figure: Wikipedia

Observations:

- Larger active space → more residual correlations left
- IM-MBPT results consistent between different active spaces
- IM-MBPT(3) results in good agreement with SR-IMSRG

OUTLOOK & CONCLUSIONS

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Conclusions:

- Demonstration of (partial) arbitrary active space decoupling.
- Post-processing with MBPT

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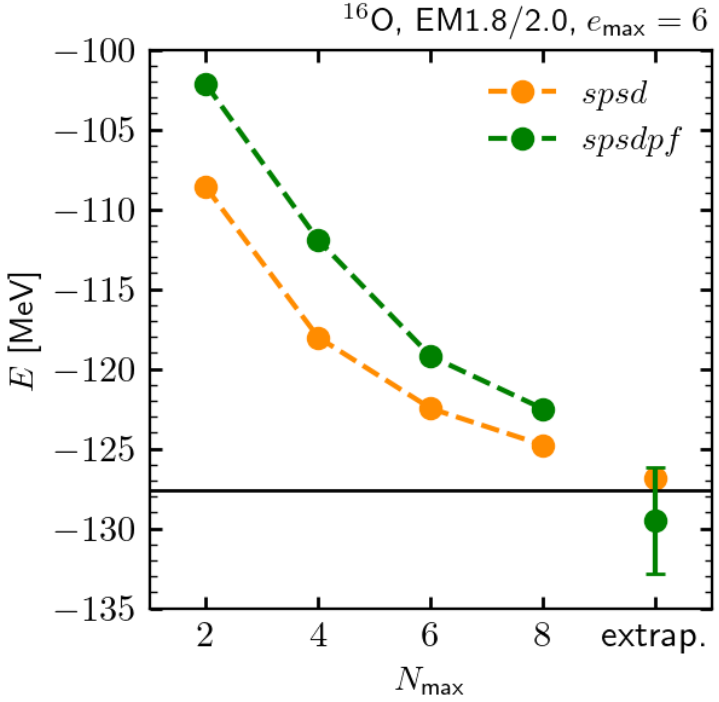

Outlook:

- IM-CI (with spectroscopy)
- Development of generators achieving more complete decoupling of the active space → decrease in post-processing model space size
- Open-shell systems with correlated reference states and study of multi-reference effects in the IMSRG flow