Recent developments in the in-medium similarity renormalization group

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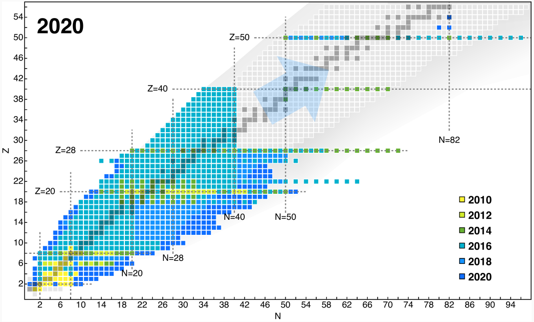
Ab initio nuclear structure



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

Interactions:

- NN and 3N interactions
- Connection to QCD → Chiral EFT

Many-body physics:

- Solve many-body Schrödinger equation in exact or systematically improvable manner

Ab initio promise:

- Predictive power
- Uncertainty quantification
- Systematic path to improvement

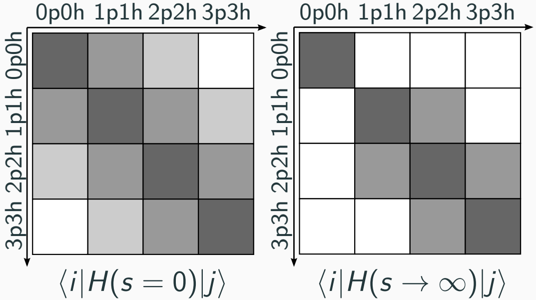
IMSRG: A conceptual overview

IMSRG evolution of Hamiltonian:

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

Unitary transformation generated by solving coupled differential equation

Start from reference state $|\Phi\rangle$ and normal order operators



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

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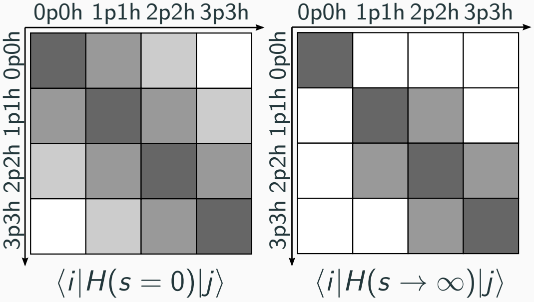
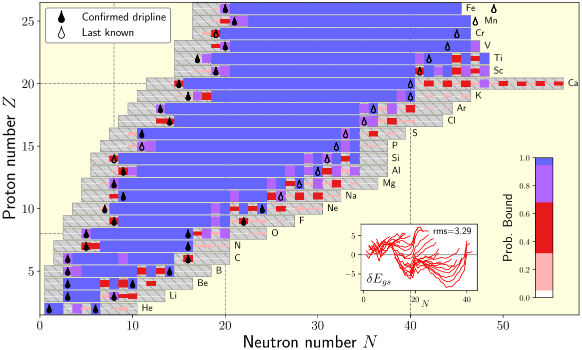
IMSRG(2):

$$H(s) = E(s) + f(s) + \Gamma(s)$$
$$O(s) = O^{(0)}(s) + O^{(1)}(s) + O^{(2)}(s)$$



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

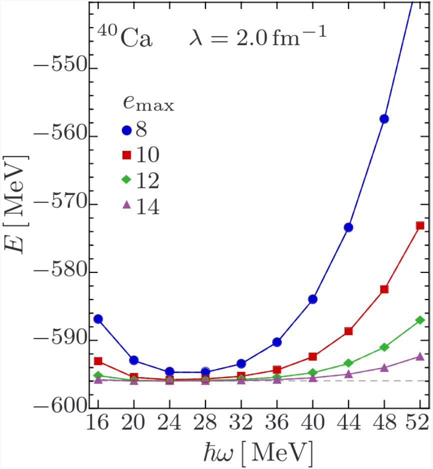
IMSRG(2): Strengths and successes



Stroberg, Holt, Schwenk, Simonis, PRL **126** (2021)

- Polynomial cost in basis size N ($\mathcal{O}(N^6)$)
- Contains all third-order diagrams
- Nonperturbative
- Can flexibly target many different quantities of interest
  - Ground-state properties
  - Spectroscopy
  - Decay matrix elements
- Multiple variants to access open-shell systems

IMSRG: Dimensions for systematic improvement



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

Basis:

- Oscillator frequency: $\hbar\Omega$
- Basis truncation: $e_{\mathrm{max}} = (2n + l)_{\mathrm{max}}$ and $E_{3\mathrm{max}} \geq e_1 + e_2 + e_3$
- Examples: HO, HF, natural orbitals (NAT)

Tichai, Müller, Vobig, Roth, PRC **99** (2019)

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

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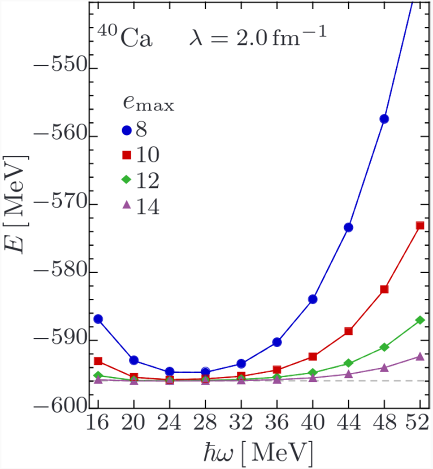

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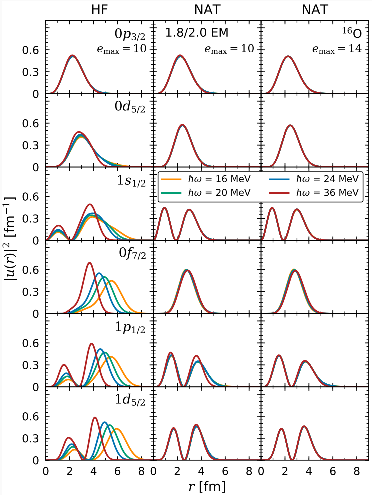
Many-body truncation:

- Correct for/relax many-body truncation
- IMSRG(2) → IMSRG(3)

MH, Tichai, Hoppe, Hebeler, Schwenk, arXiv:2102.11172

Basis improvement: Natural orbitals



Construction:

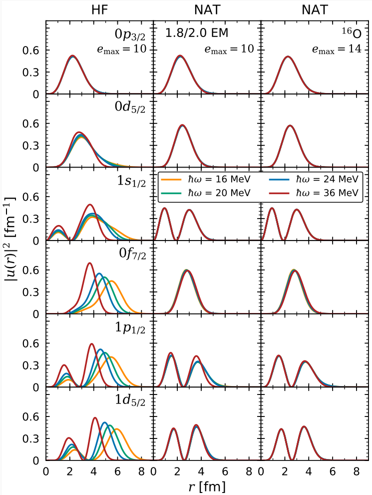
- Build density matrix in second-order perturbation theory
- Diagonalize density matrix

Properties:

- Optimizes unoccupied states
- Reduced remaining frequency dependence of basis states

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

Basis improvement: Natural orbitals



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

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Properties:

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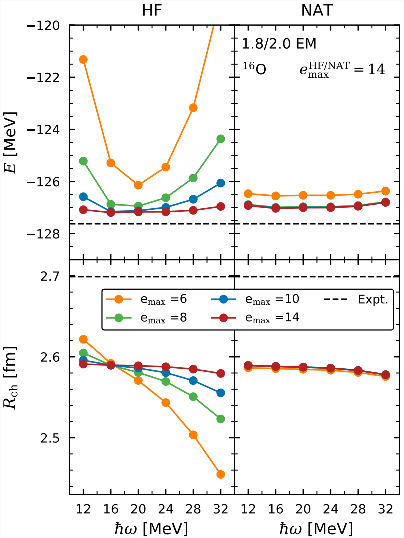
- Reduced remaining frequency dependence of basis states
- Frequency dependence of observables reduced
- Convergence behavior improved

Basis improvement: Natural orbitals

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



Application in IMSRG:

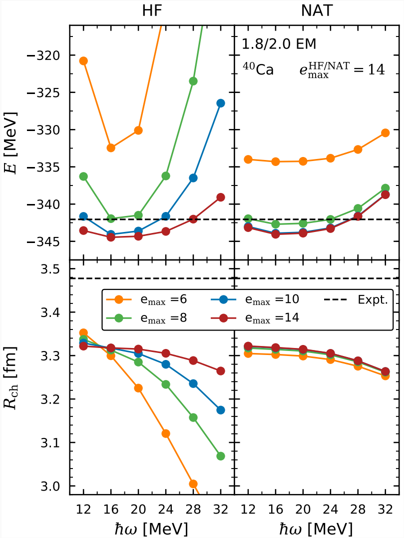
- Construct NAT in large model space
  - Here: $e_{\mathrm{max}}^{\mathrm{HF/NAT}} = 14$
- Truncate to smaller model space for IMSRG

Results:

- Improved model space convergence
- Frequency dependence reduced

Basis improvement: Natural orbitals

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



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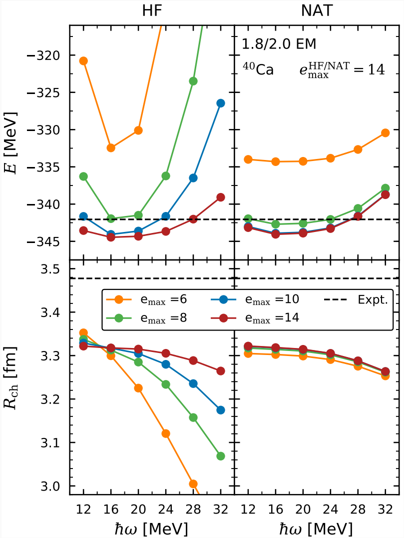
Hoppe, Tichai, MH, Hebeler, Schwenk, PRC 103 (2021)



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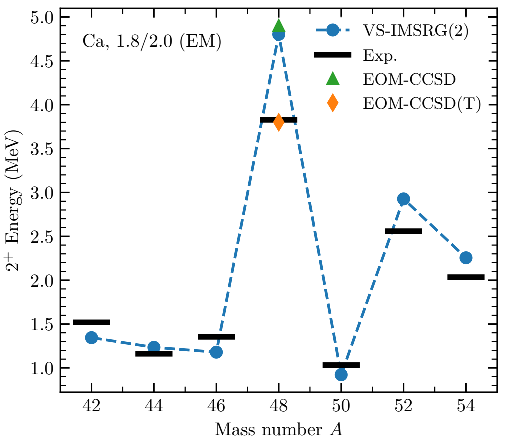
- **NAT efficiency will help converge expensive many-body calculations (IMSRG(3)!)**

Why bother with IMSRG(3)?

Triples (3p3h) are important for many relevant observables and theoretical predictions:

- 2^+ energies



Simonis, Stroberg, Hebeler, Holt, Schwenk, PRC **96** (2017)

Hagen, Jansen, Papenbrock, PRL **117** (2016)

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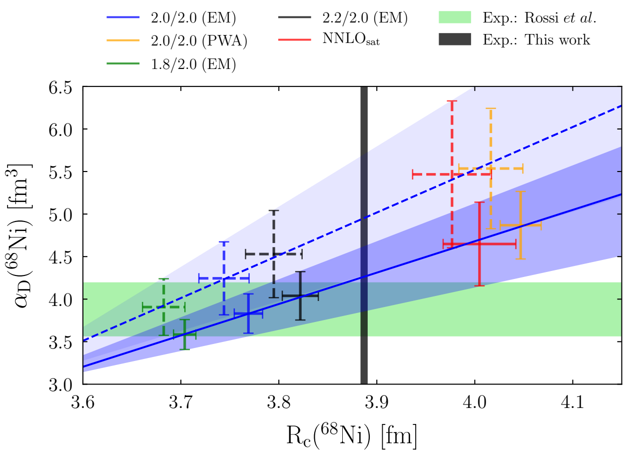
Triples (3*p*3*h*) are important for many relevant observables and theoretical predictions:

- 2^+ energies
- Dipole polarizabilities



Kaufmann *et al.*, PRL **124** (2020)

IMSRG(3)

Include three-body operators:

$$H(s) = \ldots + W(s)$$
$$O(s) = \ldots + O^{(3)}(s)$$

- Keep track of induced three-body interactions ($W(s)$)
- Can include initial residual three-body interactions
- Contains all fourth-order diagrams

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- 10 new terms in equations
- Storage cost: $\mathcal{O}(N^6)$
- Computational cost: $\mathcal{O}(N^9)$
  - Only two terms are $\mathcal{O}(N^8)$
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Goal: Approximate IMSRG(3) at lower computational cost

Approximate IMSRG(3) truncation schemes

IMSRG(3)-MP4:

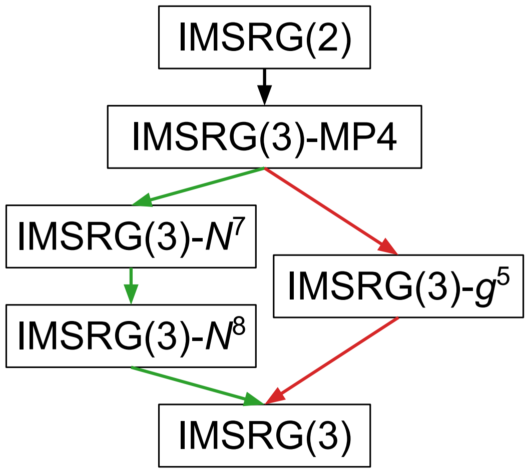
- Includes minimal terms required to be fourth-order complete

Computational organization:

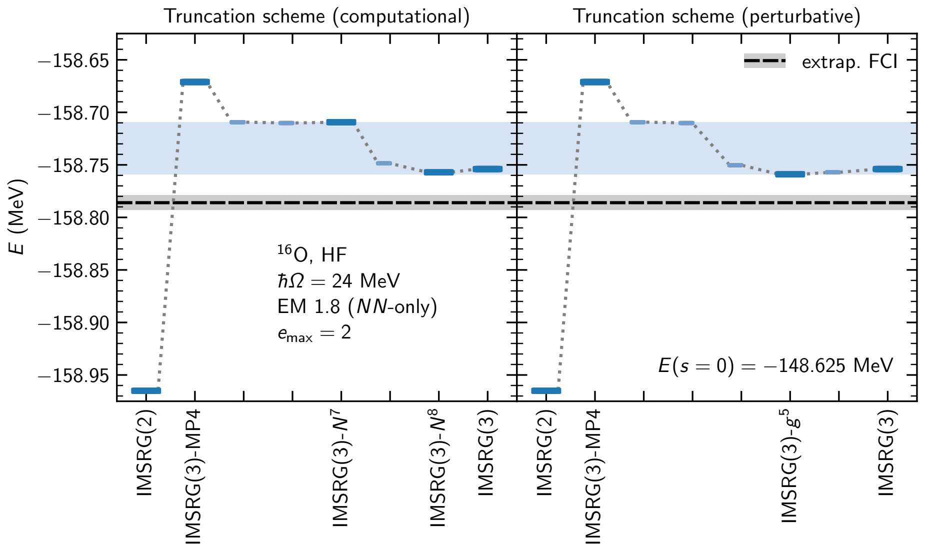
- Include terms based on computational cost

Perturbative organization:

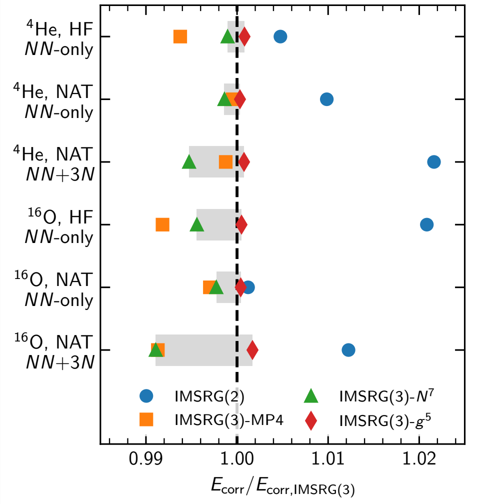
- Include terms based on perturbative importance



Application: Oxygen-16



General trends



- IMSRG(3) systematically improves over IMSRG(2) relative to exact results
- IMSRG(3)-N^7 performs better than IMSRG(2) in general
- IMSRG(3)-g^5 approximates IMSRG(3) very well ($\sim$0.1% error)
- Band between these two truncations contains IMSRG(3) results

Conclusions and outlook

Natural orbitals:

- Natural orbitals applied with great success to IMSRG
- Reduced frequency dependence and improved convergence observed

Outlook: NAT basis as robust new option for many-body calculations

IMSRG(3):

- First systematic study of full and approximate IMSRG(3) truncations performed
- Systematic improvement over IMSRG(2) relative to exact results observed

Outlook: Extend IMSRG(3) to large model spaces to study approximate truncations

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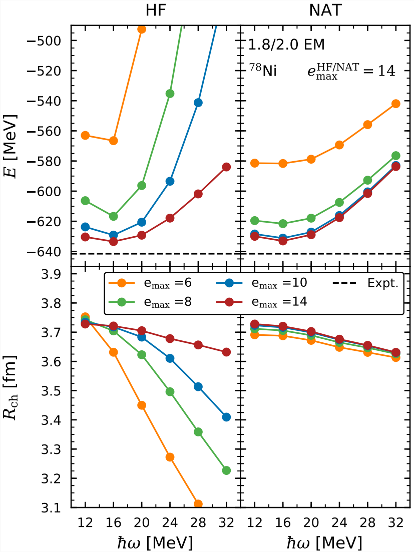
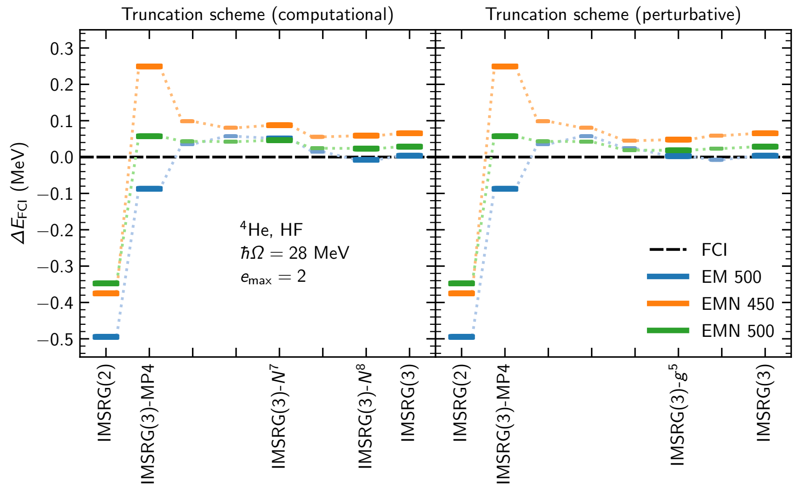
Thank you for listening!

Backup

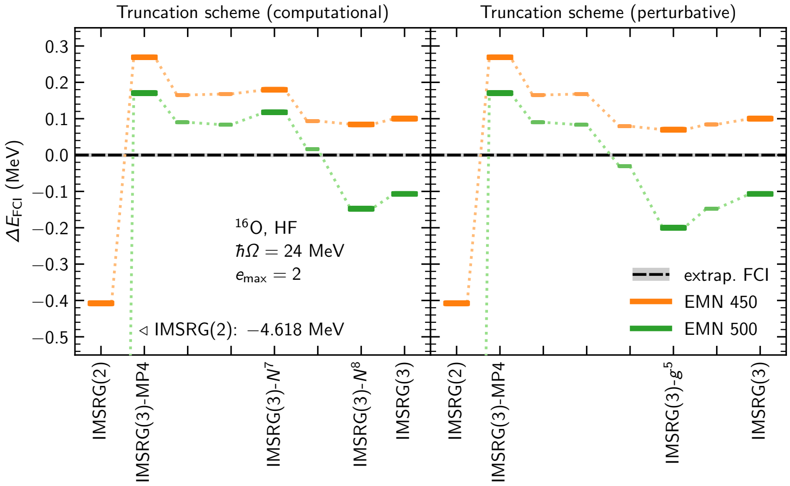
Natural orbitals in Nickel-78



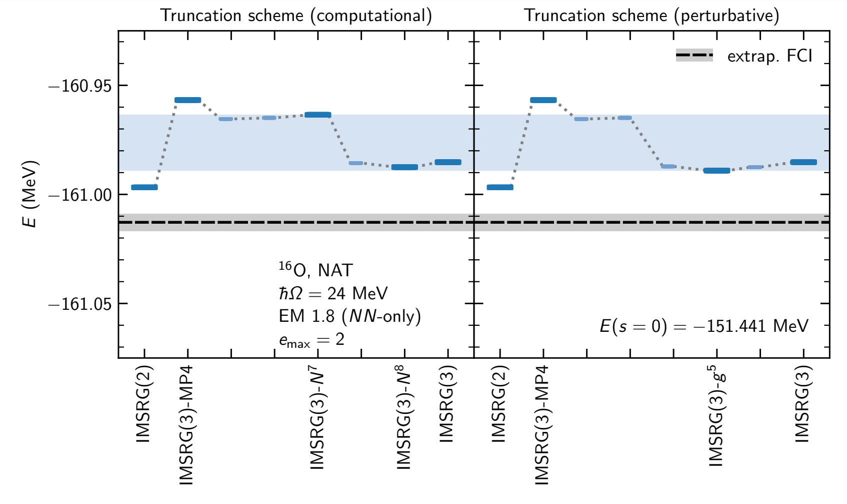
Helium-4 with harder Hamiltonians



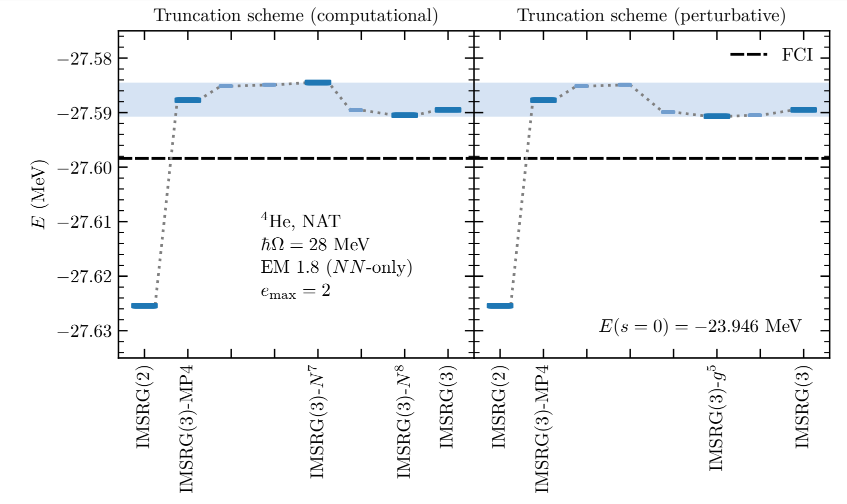
Oxygen-16 with harder Hamiltonians



Oxygen-16 (NAT)



Helium-4 (NAT)


Truncation scheme (computational)
Truncation scheme (perturbative)
FCI
−27.58
−27.59
−27.60
−27.61
−27.62
−27.63
E (MeV)
⁴He, NAT
ħΩ = 28 MeV
EM 1.8 (NN-only)
e_max = 2
E(s = 0) = −23.946 MeV
IMSRG(2)
IMSRG(3)-MP4
IMSRG(3)-N⁷
IMSRG(3)-N⁸
IMSRG(3)
IMSRG(2)
IMSRG(3)-MP4
IMSRG(3)-g⁵
IMSRG(3)

Applications with 3N interactions