In-Medium Similarity Renormalization Group

Basic Concepts, Extensions and Applications

Klaus Vobig

Institut für Kernphysik - Theoriezentrum

LOEWE
Exzellente Forschung für Hessens Zukunft

Bundesministerium für Bildung und Forschung

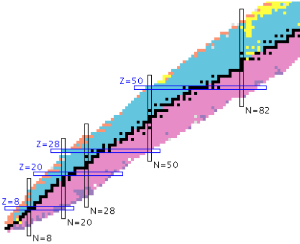
TECHNISCHE UNIVERSITÄT DARMSTADT

SFB 1245

Center for Scientific Computing Frankfurt

Motivation

- great progress with Hamiltonians derived from χEFT
- developed versatile toolbox of ab initio many-body methods
  - Importance-Truncated No-Core Shell Model (IT-NCSM)
  - Coupled Cluster (CC)
  - Many-Body Perturbation Theory
  - Self-consistent Green's functions



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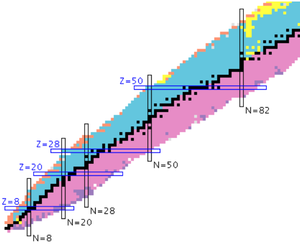
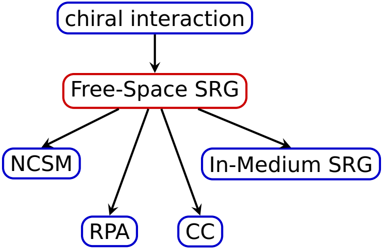


In-Medium Similarity Renormalization Group (IM-SRG)

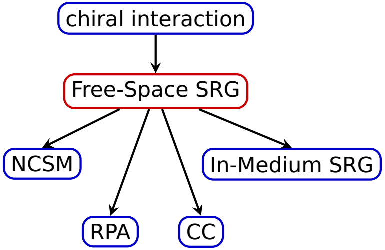
- promising novel and very flexible ab initio many-body method
- first applications: calculation of nuclear structure observables of closed-shell nuclei
  K. Tsukiyama et al., PRL 106, 222502 (2011)
- extension to multi-reference formulation for open-shell nuclei
  H. Hergert et al., PRC 90, 041302 (2014)
- construct effective interactions for, e.g., shell-model calculations
  S. Bogner et al., PRL 113, 142501 (2014)

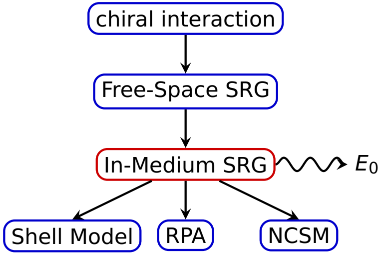
SRG-based Many-Body Methods



- tame strong short-range correlations
- "generic" decoupling of high- and low momenta in two- and three-body momentum space
- acceleration of model-space convergence

SRG-based Many-Body Methods





- tame strong short-range correlations
- "generic" decoupling of high- and low momenta in two- and three-body momentum space
- acceleration of model-space convergence

- decoupling of reference state of specific A-body system
- even further acceleration of model-space convergence
- new opportunities, e.g., valence-space interactions from ab initio treatment

SRG: Basic Concept & Formalism

- transformation towards diagonal form w.r.t. specific basis

- unitary transformation $\leftrightsquigarrow$ SRG flow equation

$$\hat{H}(s) \equiv \hat{U}^{\dagger}(s)\hat{H}(0)\hat{U}(s) \quad \leftrightsquigarrow \quad \frac{\mathrm{d}}{\mathrm{d}s}\hat{H}(s) = \left[\hat{\eta}(s)\,,\hat{H}(s)\right]$$

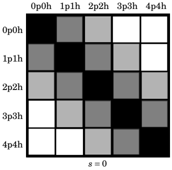
- SRG induces many-body terms up to the A-body level

$$\hat{H}(s) = \hat{H}^{[0]}(s) + \hat{H}^{[1]}(s) + \ldots + \hat{H}^{[A]}(s)$$

- antihermitian generator $\hat{\eta}(s)$ determines decoupling behavior and decoupling pattern $\rightsquigarrow$ tailor SRG for specific applications

In-Medium SRG

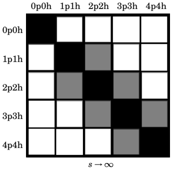
- decouple reference state $|\Phi\rangle = |i_1 i_2 \dots i_A\rangle$ from its ph-excitations $|\Phi_{i_1}^{a_1}\rangle, |\Phi_{i_1 i_2}^{a_1 a_2}\rangle, \dots$



- partition Hamiltonian $\hat{H} = \hat{H}^{\mathrm{d}} + \hat{H}^{\mathrm{od}}$, suppress "off-diagonal" part

- achieved, e.g., via Wegner generator

$$\hat{\eta}(s) \equiv \left[\hat{H}^{\mathrm{d}}(s), \hat{H}(s)\right]$$



- reference state $|\Phi\rangle$ becomes ground-state of $\hat{H}(\infty)$ with eigenvalue $\langle\Phi|\hat{H}(\infty)|\Phi\rangle$

In-Medium SRG: Key Ingredients I

- use normal-ordered form of operators throughout the evolution

$$\hat{H}(s) = E(s) + \sum_{pq} f^p_q(s) \left\{\hat{p}^\dagger \hat{q}\right\}_{|\Phi\rangle} + \frac{1}{4}\sum_{pqrs} \Gamma^{pq}_{rs}(s) \left\{\hat{p}^\dagger \hat{q}^\dagger \hat{s}\hat{r}\right\}_{|\Phi\rangle} + \dots$$

$$\hat{\eta}(s) = \sum_{pq} \eta^p_q(s) \left\{\hat{p}^\dagger \hat{q}\right\}_{|\Phi\rangle} + \frac{1}{4}\sum_{pqrs} \eta^{pq}_{rs}(s) \left\{\hat{p}^\dagger \hat{q}^\dagger \hat{s}\hat{r}\right\}_{|\Phi\rangle} + \dots$$

⇝ reference state $|\Phi\rangle$ of A-body system defines form of operators

- truncate operators at normal-ordered two-body level

- derive flow equations for $E(s)$, $f^p_q(s)$ and $\Gamma^{pq}_{rs}(s)$ from

$$\frac{\mathrm{d}}{\mathrm{d}s}\hat{H}(s) = \left[\hat{\eta}(s), \hat{H}(s)\right]$$

In-Medium SRG: Key Ingredients II

- flow equations are coupled system of first-order ordinary differential equations
- solved via numerical integration of ODE system until decoupling is reached
- typically: $\sim$ 60 million coupled differential equations
- observables have to be evolved simultaneously ($\rightsquigarrow$ $\hat{\eta}(s)$ depends on $\hat{H}(s)$)

reference states

- Single-Reference IM-SRG (SR-IM-SRG):
  - reference state is single Slater determinant from, e.g., Hartree-Fock calculation
  - applicable to closed-shell nuclei
- Multi-Reference IM-SRG (MR-IM-SRG):
  - reference state from previous NCSM or Hartree-Fock-Bogoliubov calculation
  - applicable to open-shell nuclei
  - additional terms in flow equations

NCSM & IM-NCSM

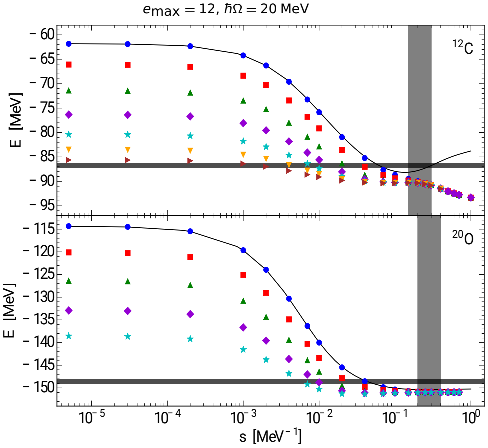
- use harmonic oscillator states with given $\hbar\Omega$ as single-particle basis
- construct Slater-determinant(s) from single-particle states
- truncate the many-body Slater-determinant basis at a maximum number of harmonic-oscillator excitation quanta N_{max}
- represent and diagonalize Hamiltonian in this model space

IM-NCSM

- use IM-SRG-evolved Hamiltonian as input for subsequent NCSM calculation
- MR-IM-SRG with NCSM reference state is used for the IM-NCSM approach
- convergence of NCSM massively improved w.r.t. N_{max}

IM-NCSM: Ground State Evolution

E. Gebrerufael et al, arXiv:1610.05254



IM-SRG zero-body part $E_0(s)$ (black solid line)

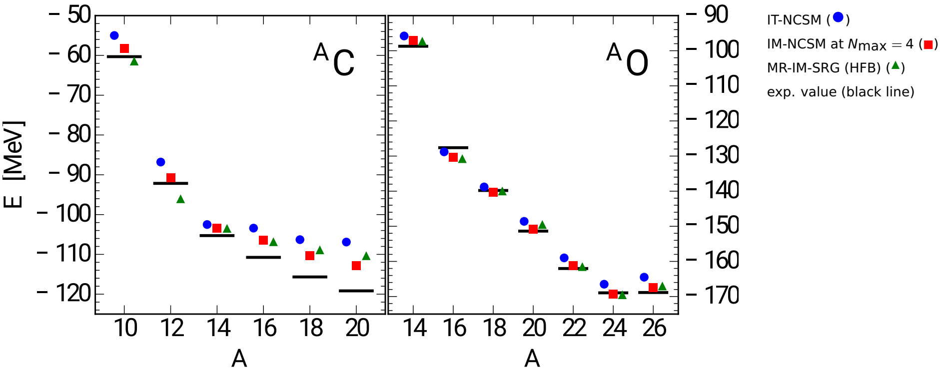
IM-NCSM $N_{max} = 0$(●), 2(■), 4(▲), 6(◆), 8(★), 10(▼), 12(▶)

IT-NCSM (horizontal band)

- NCSM convergence accelerates with increasing IM-SRG flow parameter s
- IM-SRG succesfully decouples $N_{max} = 0$ space from all basis states at higher N_{max}
- $N_{max} = 0$ eigenvalue < $E_0(s)$ $\rightsquigarrow$ reference state not $N_{max} = 0$ eigenstate
- effects of neglected many-body contributions beyond normal-ordered two-body level

IM-NCSM: Ground States Carbon & Oxygen Chain

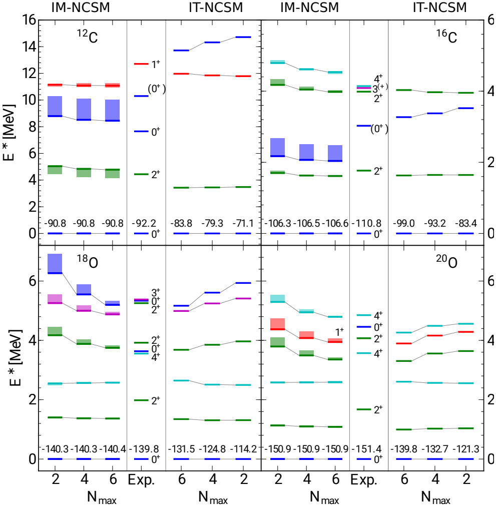
E. Gebrerufael et al, arXiv:1610.05254



- very good agreement between methods for oxygen (deviations ∼ 2%)
- larger method uncertainties for carbon isotopes, especially ^{12}C

IM-NCSM: Spectra

E. Gebrerufael et al, arXiv:1610.05254

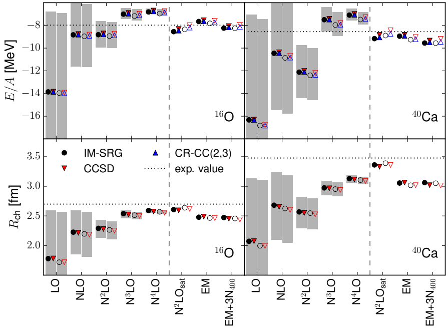


IM-NCSM bands: uncertainty estimate

- good agreement for well converged states
- slow convergence w.r.t. N_{max}
  ⇝ dominant contributions from outside $N_{\mathrm{max}} = 0$ space
- surprising behavior of 0^+ state in ^{12}C and ^{16}C

New Chiral Interactions: Benchmarks

paper in preparation



theoretical error bars in gray

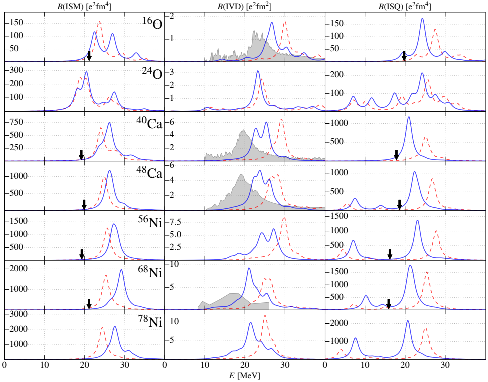
$\alpha = 0.04\ \text{fm}^4$ (open)

$\alpha = 0.08\ \text{fm}^4$ (solid)

- ground-state energies and charge radii from the IM-SRG and CC
- very good agreement of many-body methods
- characteristic pattern from LO to N^4LO
- compared to NN of E. & M.
  - more attractive 3N forces necesssary (N^3LO,N^4LO)
  - radii improved, still underestimated

IM-SRG & SRPA: Transition Strengths

R. Trippel, doctoral thesis



N^2LO_{sat} (blue line)

$NN_{EM}+3N_{400}$ (dashed red line)

exp. centroid (arrow) or spectra (gray)

- SRPA: 2p2h EoM approach
  ⇝ description of collective motions
- IM-SRG-evolved Hamiltonian as input
  ⇝ improved physical content of reference state
- transition strengths of high experimental interest
- good qualitiative agreement between experiment and theory

Epilogue

- **Thanks to my group**
  - S. Alexa, S. Dentinger, **E. Gebrerufael**, T. Hüther, L. Kreher, L. Mertes, R. Roth, S. Schulz, H. Spielvogel, H. Spiess, C. Stumpf, A. Tichai, **R. Trippel**, R. Wirth, T. Wolfgruber

    Institut für Kernphysik, TU Darmstadt

- **Thank you for your attention!**

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JURECA — JÜLICH FORSCHUNGSZENTRUM

LOEWE-CSC — Center for Scientific Computing Frankfurt

LICHTENBERG — HRZ Hochschulrechenzentrum

SFB 1245

Deutsche Forschungsgemeinschaft DFG

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HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung