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

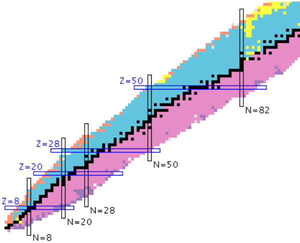
SFB 1245

CSC Center for Scientific Computing Frankfurt

Motivation

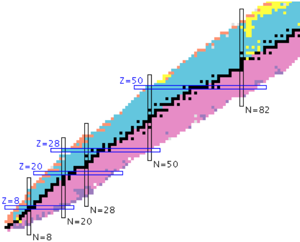
- great progress with Hamiltonians derived from χEFT

- developed versatile toolbox of ab initio many-body methods for medium-/heavy-mass nuclei:
  - Coupled Cluster (CC) (⇝ lectures of M. Hjorth-Jensen)
  - Many-Body Perturbation Theory (⇝ lectures of M. Hjorth-Jensen)
  - Self-consistent Green's functions (⇝ lectures of V. Soma)



Motivation

- great progress with Hamiltonians derived from χEFT
- developed versatile toolbox of ab initio many-body methods for medium-/heavy-mass nuclei:
  - Coupled Cluster (CC) (⇝ lectures of M. Hjorth-Jensen)
  - Many-Body Perturbation Theory (⇝ lectures of M. Hjorth-Jensen)
  - Self-consistent Green's functions (⇝ lectures of V. Soma)



In-Medium Similarity Renormalization Group (IM-SRG)

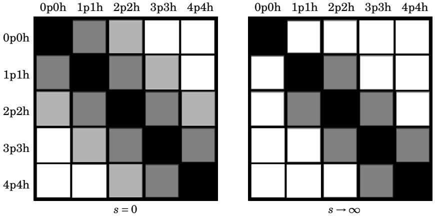
- promising novel method
- great advantage: flexibility of formulation
- first applications: calculation of nuclear structure observables of closed-shell nuclei

  H. Hergert et al., PRC 87, 034307 (2013)
- 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 (⇝ seminar C. Stumpf)

  S. Bogner et al., PRL 113, 142501 (2014)
- excited states

- 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 via continuous unitary transformation

$$\hat{H}(s) \equiv \hat{U}^\dagger(s)\hat{H}(0)\hat{U}(s)$$

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

Concept & Formalism

- unitary transformation $\rightsquigarrow$ efficient SRG flow equation

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

- anti-hermitian generator $\hat{\eta} = -\hat{U}^{\dagger}(s)\left(\frac{\mathrm{d}}{\mathrm{d}s}\hat{U}(s)\right)$ (more later)

Concept & Formalism

- unitary transformation $\leftrightsquigarrow$ efficient SRG flow equation

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

- anti-hermitian generator $\hat{\eta} = -\hat{U}^\dagger(s)\left(\frac{\mathrm{d}}{\mathrm{d}s}\hat{U}(s)\right)$ (more later)

- use normal-ordered form of operators throughout the evolution

$$\hat{H}(s) = E(s) + \sum_{pq} f^p_q(s)\,\{\hat{p}^\dagger\hat{q}\} + \frac{1}{4}\sum_{pqrs}\Gamma^{pq}_{rs}(s)\,\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \ldots$$

$$\hat{\eta}(s) = \sum_{pq} \eta^p_q(s)\,\{\hat{p}^\dagger\hat{q}\} + \frac{1}{4}\sum_{pqrs}\eta^{pq}_{rs}(s)\,\{\hat{p}^\dagger\hat{q}^\dagger\hat{s}\hat{r}\} + \ldots$$

note difference to free-space SRG!

- truncate at normal-ordered two-body level (NO2B)

- evaluate commutator using Wick's theorem

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

Flow Equations

$$\frac{\mathrm{d}}{\mathrm{d}s}E(s) = \sum_{pq} (n_p - n_q)\ \eta^p_q(s)\ f^q_p(s) + \frac{1}{4} \sum_{pqrs} \left(\eta^{pq}_{rs}(s)\ \Gamma^{rs}_{pq}(s)\ n_p n_q \bar{n}_r \bar{n}_s - [\eta \leftrightarrow \Gamma]\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}s}f^1_2(s) = \sum_p \left(\eta^1_p\ f^p_2\ - [\eta \leftrightarrow f]\right) + \ldots$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\Gamma^{12}_{34}(s) = \sum_p \left(\left(\eta^1_p\ \Gamma^{p2}_{34} - f^1_p\ \eta^{p2}_{34}\right) - [1 \leftrightarrow 2]\right) - \ldots$$

- flow equations are coupled system of first-order ordinary differential equations
- solved via numerical integration of ODE system until decoupling is reached
- typically: ~ 62 million coupled differential equations
- highly efficient implementation in C using BLAS and exploitation of physical symmetries (e.g. spherical symmetry)
- observables have to be evolved simultaneously ($\rightsquigarrow \hat{\eta}(s)$ depends on $\hat{H}(s)$)

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

- alternative formulation: Magnus expansion

$$\frac{\mathrm{d}}{\mathrm{d}s}E(s) = \sum_{pq} (n_p - n_q)\ \eta^p_q(s)\ f^q_p(s) + \frac{1}{4} \sum_{pqrs} \left(\eta^{pq}_{rs}(s)\ \Gamma^{rs}_{pq}(s)\ n_p n_q \bar{n}_r \bar{n}_s - [\eta \leftrightarrow \Gamma]\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}s}f^1_2(s) = \sum_p \left(\eta^1_p\ f^p_2\ - [\eta \leftrightarrow f]\right) + \dots$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\Gamma^{12}_{34}(s) = \sum_p \left(\left(\eta^1_p\ \Gamma^{p2}_{34} - f^1_p\ \eta^{p2}_{34}\right) - [1 \leftrightarrow 2]\right) - \dots$$

- flow equations are coupled system of first-order ordinary differential equations
- solved via numerical integration of ODE system until decoupling is reached
- typically: ~ 62 million coupled differential equations
- highly efficient implementation in C using BLAS and exploitation of physical symmetries (e.g. spherical symmetry)
- observables have to be evolved simultaneously ($\rightsquigarrow \hat{\eta}(s)$ depends on $\hat{H}(s)$)
- alternativ

nonlinear algebraic equations for cluster amplitudes (CC)

↕

coupled differential equations for matrix elements (IM-SRG)

Generators

- choice of generator $\hat{\eta} \longleftrightarrow$ desired behavior

- determines decoupling behavior and decoupling pattern $\rightsquigarrow$ tailor IM-SRG for specific applications via choice of generator

- identify "off-diagonal" part of Hamiltonian:

$$\langle \Phi | \hat{H} | \Phi_{i_1}^{a_1} \rangle = f_{a_1}^{i_1}$$
$$\langle \Phi | \hat{H} | \Phi_{i_1 i_2}^{a_1 a_2} \rangle = \Gamma_{a_1 a_2}^{i_1 i_2}$$

- several generator types, e.g. , Wegner:

$$\hat{\eta}(s) = \left[\hat{H}(s), \hat{H}^{\text{od}}(s)\right]$$

- improved numerical characteristics and efficiencies: White and imaginary-time generator

Generators

- choice of generator $\hat{\eta} \longleftrightarrow$ desired behavior

- determines decoupling behavior and decoupling pattern ⇝ tailor IM-SRG for specific applications via choice of generator

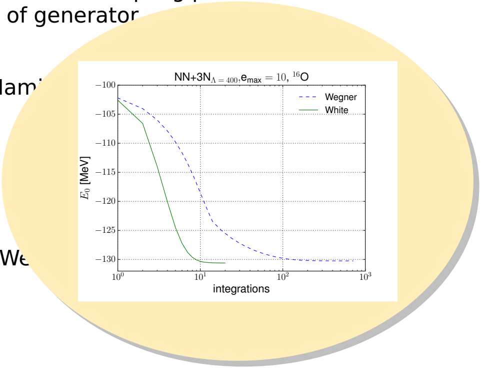
- identify "off-diagonal" part of Ham

$$\langle\Phi|\hat{H}|\Phi_{i_1}^{a_1}\rangle = f_{a_1}^{i_1}$$

$$\langle\Phi|\hat{H}|\Phi_{i_1 i_2}^{a_1 a_2}\rangle = \Gamma_{a_1 a_2}^{i_1 i_2}$$

- several generator types, e.g. , We

$$\hat{\eta}(s) = \left[\hat{H}(s), \hat{H}^{\text{od}}(s)\right]$$



- improved numerical characteristics and efficiencies: White and imaginary-time generator

previous chiral NN+3N interactions:

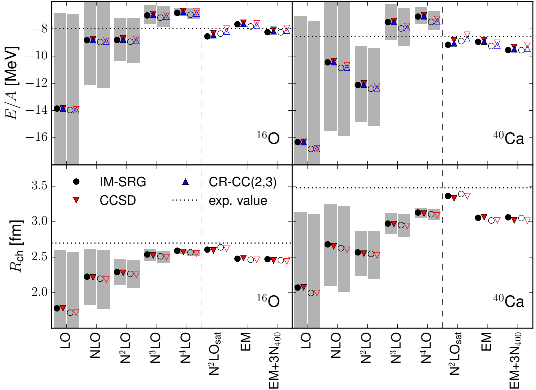
- significant overestimation of binding energies beyond oxygen chain — S. Binder et al., PLB 736, 119 (2014)
- underestimation of radii

NN at N^3LO: D. R. Entem et al., PRC 68, 041001 (2003)

3N at N^2LO with $\Lambda = 400$ MeV: R. Roth et al., PRL 109, 052501 (2012)

next-generation interactions

- N^2LO_{sat} interaction — A. Ekström et al., PRC 91, 051301 (2015)
  - include information from heavier systems for LEC fitting
- improved chiral interaction — E. Epelbaum et al., Eur. Phys. J. A 51, 53 (2015); S. Binder et al., PRC 93, 044002 (2016)
  - up to N^4LO
  - developed within LENPIC collaboration
  - semi-local regulators
  - study of order-by-order convergence
  - systematically assess χEFT uncertainties



- agreement of many-body methods
- characteristic pattern from LO to N^{4}LO
- compared to NN of E. & M.
  - more attractive 3N forces necesssary (N^{3}LO,N^{4}LO)
  - radii improved, still underestimated

- theoretical error bars in gray

S. Binder et al., PRC 93, 044002 (2016)
(⇝ lectures of P. Maris)

- 0.04 fm^4 (open)
- 0.08 fm^4 (solid)

summary

- employ unitary transformation for decoupling of reference state $|\Phi\rangle$
- solve coupled system of ordinary differential equations
- flexible formulation
- competitive with most advanced Coupled Cluster methods

outlook

- study electromagnetic observables
- asses induced three-body effects
- overcome restriction to even-even nuclei

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, K. Vobig, R. Wirth, T. Wolfgruber
    Institut für Kernphysik, TU Darmstadt

- **Thank you for your attention!**

COMPUTING TIME

JURECA	LOEWE-CSC	LICHTENBERG
JÜLICH FORSCHUNGSZENTRUM	CSC Center for Scientific Computing Frankfurt	HRZ Hochschulrechenzentrum

SFB 1245

TECHNISCHE UNIVERSITÄT DARMSTADT

Deutsche Forschungsgemeinschaft
DFG

LOEWE
Exzellente Forschung für Hessens Zukunft

HELMHOLTZ GEMEINSCHAFT

Bundesministerium für Bildung und Forschung