Multi-Reference IM-SRG for Nuclei

Heiko Hergert

National Superconducting Cyclotron Laboratory Michigan State University





- The Similarity Renormalization Group
- In-Medium SRG
- Multi-Reference In-Medium SRG
- Ground States of Closed- and Open-Shell Nuclei
- Next Steps
- Conclusions

Prelude: Similarity Renormalization Group

Review:

S. Bogner, R. Furnstahl, and A. Schwenk, Prog. Part. Nucl. Phys. 65 (2010), 94

E. Anderson, S. Bogner, R. Furnstahl, and R. Perry, Phys. Rev. C82 (2011), 054001
E. Jurgenson, P. Navratil, and R. Furnstahl, Phys. Rev. C83 (2011), 034301
R. Roth, S. Reinhardt, and H. H., Phys. Rev. C77 (2008), 064003
H. H. and R. Roth, Phys. Rev. C75 (2007), 051001

Similarity Renormalization Group

Basic Concept

continuous unitary transformation of the Hamiltonian to banddiagonal form w.r.t. a given "uncorrelated" many-body basis

• flow equation for Hamiltonian $H(s) = U(s)HU^{\dagger}(s)$:

$$\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right], \quad \eta(s) = \frac{dU(s)}{ds}U^{\dagger}(s) = -\eta^{\dagger}(s)$$

• choose $\eta(s)$ to achieve desired behavior, e.g.,

$$\eta(\mathbf{s}) = \left[\mathbf{H}_{\mathbf{d}}(\mathbf{s}), \mathbf{H}_{\mathbf{od}}(\mathbf{s}) \right]$$

to suppress (suitably defined) off-diagonal Hamiltonian

• consistent evolution for all observables of interest



In-Medium SRG

S. K. Bogner, H. H., T. Morris, A. Schwenk, and K. Tuskiyama, to appear in Phys. Rept. H. H., S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk, Phys. Rev. C 87, 034307 (2013)

K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. Lett. 106, 222502 (2011)

Solving the Flow Equation



• operator flow equation:

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

- encodes information for all systems described by H
- ("arbitrarily") complex unitary transformation to solve everything at once
- truncation / organization scheme
 - introduces restrictions (particle number, ...), uncertainties
- basis (operator algebra and/or Hilbert space)
- generator
 - introduce information from target system (e.g. reference state) to optimize transformation, reduce uncertainties

Decoupling in A-Body Space



 (\mathfrak{S})

G

Normal Ordering



- second quantization: $A_{I_1...I_N}^{k_1...k_N} = a_{k_1}^{\dagger} \dots a_{k_N}^{\dagger} a_{I_N} \dots a_{I_1}$
- particle- and hole density matrices:

$$\lambda_{l}^{k} = \left\langle \Phi \middle| A_{l}^{k} \middle| \Phi \right\rangle \longrightarrow n_{k} \delta_{l}^{k}, \quad n_{k} \in \{0, 1\}$$

$$\xi_{l}^{k} = \lambda_{l}^{k} - \delta_{l}^{k} \longrightarrow -\overline{n}_{k} \delta_{l}^{k} \equiv -(1 - n_{k}) \delta_{l}^{k}$$

• define normal-ordered operators recursively:

$$\begin{aligned} A_{l_1...l_N}^{k_1...k_N} &=: A_{l_1...l_N}^{k_1...k_N} :+ \lambda_{l_1}^{k_1} :A_{l_2...l_N}^{k_2...k_N} :+ \text{singles} \\ &+ \left(\lambda_{l_1}^{k_1} \lambda_{l_2}^{k_2} - \lambda_{l_2}^{k_1} \lambda_{l_1}^{k_2}\right) :A_{l_3...l_N}^{k_3...k_N} :+ \text{doubles} + \dots \end{aligned}$$

• algebra is simplified significantly because

$$\langle \Phi | : A_{I_1...I_N}^{k_1...k_N} : | \Phi \rangle = 0$$

 Wick's theorem gives simplified expansions (fewer terms!) for products of normal-ordered operators

Normal-Ordered Hamiltonian



Normal-Ordered Hamiltonian

W



two-body formalism with in-medium contributions from three-body interactions

Decoupling in A-Body Space



S

aim: decouple reference state $|\Phi\rangle$ (0p-0h) from excitations

Decoupling in A-Body Space



• define off-diagonal Hamiltonian (suppressed by IM-SRG flow):

$$H_{od} \equiv f_{od} + \Gamma_{od}, \quad f_{od} \equiv \sum_{ph} f_h^p : A_h^p : + \text{H.c.}, \quad \Gamma_{od} \equiv \frac{1}{4} \sum_{pp'hh'} \Gamma_{hh'}^{pp'} : A_{hh'}^{pp'} : + \text{H.c.}$$

construct generator

Choice of Generator



• Wegner:
$$\eta' = [H_d, H_{od}]$$

• White: (J. Chem. Phys. 117, 7472)

$$\eta'' = \sum_{ph} \frac{f_h^p}{\Delta_h^p} : A_h^p : +\frac{1}{4} \sum_{pp'hh'} \frac{\Gamma_{hh'}^{pp'}}{\Delta_{hh'}^{pp'}} : A_{hh'}^{pp'} : -\text{H.c.}$$

$$\Delta_h^p, \Delta_{hh'}^{pp'} : \text{approx. 1p1h, 2p2h excitation energies}$$

• "imaginary time": (Morris, Bogner)

$$\eta^{III} = \sum_{ph} \operatorname{sgn}\left(\Delta_{h}^{p}\right) f_{h}^{p} : A_{h}^{p} : + \frac{1}{4} \sum_{pp'hh'} \operatorname{sgn}\left(\Delta_{hh'}^{pp'}\right) \Gamma_{hh'}^{pp'} : A_{hh'}^{pp'} : - \text{H.c.}$$

- off-diagonal matrix elements are suppressed like $e^{-\Delta^2 s}$ (Wegner), e^{-s} (White), and $e^{-|\Delta|s}$ (imaginary time)
- g.s. energies (s $\rightarrow \infty$) differ by $\ll 1\%$

IM-SRG(2) Flow Equations





IM-SRG(2): truncate ops. at two-body level

H. Hergert - Long

IM-SRG(2) Flow Equations





Decoupling





Multi-Reference IM-SRG

H. H., in preparation

H. H., S. Bogner, T. Morris, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. C 90, 041302 (2014)

H. H., S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett 110, 242501 (2013)



- generalized Wick's theorem for arbitrary reference states (Kutzelnigg & Mukherjee)
- define irreducible n-body density matrices of reference state:

$$\rho_{mn}^{kl} = \lambda_{mn}^{kl} + \lambda_m^k \lambda_n^l - \lambda_n^k \lambda_m^l$$
$$\rho_{lmn}^{ijk} = \lambda_{lmn}^{ijk} + \lambda_l^i \lambda_{mn}^{jk} + \lambda_l^i \lambda_m^{jk} \lambda_n^k + \text{permutations}$$

• irreducible densities give rise to additional contractions:

$$: A_{cd...}^{ab...} :: A_{mn...}^{kl...} : \longrightarrow \lambda_{mn}^{ab}$$
$$: A_{cd...}^{ab...} :: A_{mn...}^{kl...} : \longrightarrow \lambda_{cm}^{ab}$$

Decoupling Revisited



$$\left\langle \begin{array}{l} p \\ s \end{array} \middle| H \middle| \Phi \right\rangle \sim \bar{n}_{p} n_{s} f_{s}^{p}, \sum_{kl} f_{l}^{k} \lambda_{pl}^{sk}, \sum_{klmn} \Gamma_{mn}^{kl} \lambda_{pmn}^{skl}, \dots \\ p_{st}^{pq} \middle| H \middle| \Phi \right\rangle \sim \bar{n}_{p} \bar{n}_{q} n_{s} n_{t} \Gamma_{st}^{pq}, \sum_{kl} \Gamma_{sl}^{pk} \lambda_{ql}^{tk}, \sum_{kl} f_{l}^{k} \lambda_{pql}^{stk}, \sum_{klmn} \Gamma_{mn}^{kl} \lambda_{pqmn}^{stkl}, \dots \\ p_{stu}^{pqr} \middle| H \middle| \Phi \right\rangle \sim \dots$$

- truncation in irreducible density matrices based on, e.g.,
 - number of correlated vs. total pairs, triples, ... (caveat: highly collective reference states)
 - perturbative analysis (e.g. for shell-model like states)
- verify for chosen multi-reference state when possible

Generators





- White generator: small energy denominators due to neardegeneracies
- imaginary time generator: sign choice depends on approximate energies
- definition of H^{od} subject to density truncations



• consider unitary variations of the energy functional

$$\boldsymbol{E}(\boldsymbol{s}) = \left\langle \left. \boldsymbol{\Phi} \right| \boldsymbol{H}(\boldsymbol{s}) \left| \boldsymbol{\Phi} \right. \right\rangle$$

 define generator as the residual of the irreducible Brillouin condition (= gradient of E)

$$\eta_{r}^{p} \equiv \left\langle \Phi \right| \left[: A_{r}^{p} :, H \right] \left| \Phi \right\rangle$$
$$\eta_{rs}^{pq} \equiv \left\langle \Phi \right| \left[: A_{rs}^{pq} :, H \right] \left| \Phi \right\rangle$$

- fixed point ($\eta = 0$) is reached when IBC is satisfied, energy stationary (cf. ACSE approach of Mazziotti et al.)
- Brillouin generator depends linearly on λ_s^p , λ_{st}^{pq} , λ_{stu}^{pqr} , higher irreducible density matrices are not required

Brillouin Generator





 norm of Brillouin generator decays monotonically (approximation: 2B "particle-hole"-like term switched off, 3B density not yet implemented)

use in Magnus formulation of MR-IM-SRG

Multi-Reference Flow Equations



0-body flow:

$$\begin{aligned} \frac{dE}{ds} &= \sum_{ab} (n_a - n_b) \left(\eta_b^a f_a^b - f_b^a \eta_a^b \right) + \frac{1}{4} \sum_{abcd} \left(\eta_{cd}^{ab} \Gamma_{ab}^{cd} - \Gamma_{cd}^{ab} \eta_{ab}^{cd} \right) n_a n_b \bar{n}_c \bar{n}_d \\ &+ \frac{1}{4} \sum_{abcd} \left(\frac{d}{ds} \Gamma_{cd}^{ab} \right) \lambda_{cd}^{ab} + \frac{1}{4} \sum_{abcdklm} \left(\eta_{cd}^{ab} \Gamma_{am}^{kl} - \Gamma_{cd}^{ab} \eta_{am}^{kl} \right) \lambda_{cdm}^{bkl} \end{aligned}$$

1-body flow:

$$\begin{split} \frac{d}{ds} f_{2}^{1} &= \sum_{a} \left(\eta_{a}^{1} f_{2}^{a} - f_{a}^{1} \eta_{2}^{a} \right) + \sum_{ab} \left(\eta_{b}^{a} \Gamma_{a2}^{b1} - f_{b}^{a} \eta_{a2}^{b1} \right) (n_{a} - n_{b}) \\ &+ \frac{1}{2} \sum_{abcdef} \left(\eta_{bc}^{1a} \Gamma_{2a}^{bc} - \Gamma_{bc}^{1a} \eta_{2a}^{bc} \right) (n_{a} \bar{n}_{b} \bar{n}_{c} + \bar{n}_{a} n_{b} n_{c}) \\ &+ \frac{1}{4} \sum_{abcde} \left(\eta_{bc}^{1a} \Gamma_{2a}^{de} - \Gamma_{bc}^{1a} \eta_{2a}^{de} \right) \lambda_{bc}^{de} + \sum_{abcde} \left(\eta_{bc}^{1a} \Gamma_{2d}^{be} - \Gamma_{bc}^{1a} \eta_{2d}^{be} \right) \lambda_{cd}^{ae} \\ &- \frac{1}{2} \sum_{abcde} \left(\eta_{2b}^{1a} \Gamma_{ae}^{cd} - \Gamma_{2b}^{1a} \eta_{ae}^{cd} \right) \lambda_{be}^{cd} + \frac{1}{2} \sum_{abcde} \left(\eta_{2b}^{1a} \Gamma_{de}^{bc} - \Gamma_{2b}^{1a} \eta_{de}^{bc} \right) \lambda_{de}^{ac} \end{split}$$

H. Hergert - ESNT Workshop "Near-Degenerate Systems in Nuclear Structure and Quantum Chemistry from Ab Initio Methods", CEA Saclay, 03/31/2015



2-body flow:

$$\frac{d}{ds}\Gamma_{34}^{12} = \sum_{a} \left(\eta_{a}^{1}\Gamma_{34}^{a2} + \eta_{a}^{2}\Gamma_{34}^{1a} - \eta_{3}^{a}\Gamma_{a4}^{12} - \eta_{4}^{a}\Gamma_{3a}^{12} - f_{a}^{1}\eta_{34}^{a2} - f_{a}^{2}\eta_{34}^{1a} + f_{3}^{a}\eta_{a4}^{12} + f_{4}^{a}\eta_{3a}^{12} \right) \\
+ \frac{1}{2}\sum_{ab} \left(\eta_{ab}^{12}\Gamma_{34}^{ab} - \Gamma_{ab}^{12}\eta_{34}^{ab} \right) (1 - n_{a} - n_{b}) \\
+ \sum_{ab} (n_{a} - n_{b}) \left(\left(\eta_{3b}^{1a}\Gamma_{4a}^{2b} - \Gamma_{3b}^{1a}\eta_{4a}^{2b} \right) - \left(\eta_{3b}^{2a}\Gamma_{4a}^{1b} - \Gamma_{3b}^{2a}\eta_{4a}^{1b} \right) \right)$$

two-body flow unchanged, O(N⁶) scaling preserved

Particle-Number Projected HFB State

 HFB ground state is a superposition of states with different particle number:

$$\Psi \rangle = \sum_{A=N,N\pm2,...} c_A |\Psi_A \rangle, \quad |\Psi_N \rangle \equiv P_N |\Psi \rangle \equiv \frac{1}{2\pi} \int_0^{2\pi} d\phi \, e^{i\phi(\hat{N}-N)} |\Psi \rangle$$

• calculate irreducible densities (project only once), e.g.,

$$\lambda_{I}^{k} = \frac{\left\langle \Psi \middle| A_{I}^{k} P_{N} \middle| \Psi \right\rangle}{\left\langle \Psi \middle| \Psi \right\rangle}, \quad \lambda_{mn}^{kl} = \frac{\left\langle \Psi \middle| A_{mn}^{kl} P_{N} \middle| \Psi \right\rangle}{\left\langle \Psi \middle| \Psi \right\rangle} - \lambda_{m}^{k} \lambda_{m}^{l} + \lambda_{n}^{k} \lambda_{m}^{l}$$

• work in natural orbitals (= HFB canonical basis):

$$\lambda_l^k = n_k \delta_l^k \left(= v_k^2 \delta_l^k \right) , \quad 0 \le n_k \le 1$$

• in NO basis, λ_{mn}^{kl} , λ_{nop}^{klm} require only 2N², 3N³ storage

Ground States of Closed and Open-Shell Nuclei

H. H., in preparation

H. H., S. Bogner, T. Morris, S. Binder, A. Calci, J. Langhammer, R. Roth, Phys. Rev. C 90, 041302 (2014)

H. H., S. Binder, A. Calci, J. Langhammer, and R. Roth, Phys. Rev. Lett 110, 242501 (2013)

H. H., S. K. Bogner, S. Binder, A. Calci, J. Langhammer, R. Roth, and A. Schwenk, Phys. Rev. C 87, 034307 (2013)



Initial Hamiltonian

- NN: chiral interaction at N³LO (Entern & Machleidt)
- 3N: chiral interaction at N²LO (c_D, c_E fit to ³H, ⁴He energies, β decay)

SRG-Evolved Hamiltonians

- NN + 3N-induced: start with initial NN Hamiltonian, keep two- and three-body terms
- NN + 3N-full: start with initial NN + 3N Hamiltonian, keep two- and three-body terms

Results: Oxygen Chain





- Multi-Reference IM-SRG with number-projected Hartree-Fock-Bogoliubov as reference state (pairing correlations)
- consistent results from different many-body methods

Two-Neutron Separation Energies



- differential observables (S_{2n}, spectra,...) filter out interaction components that cause overbinding
- predict flat trends for g.s.
 energies/S_{2n} beyond ⁵⁴Ca
 await experimental data
- ⁵²Ca, ⁵⁴Ca robustly magic due to 3N interaction
- no continuum coupling yet, other S_{2n} uncertainties < 1MeV

ucture and Quantum Chemistry from Ab Initio Methods", CEA Saclay, 03/31/2015

Two-Neutron Separation Energies



- flat trends for g. s. energies and S_{2n} (similar to Ca)
- deformation instability in ^{64,66}Ni calculations - issue with "shell" structure
- further evidence from 3N cutoff variation
- no continuum coupling yet, other S_{2n} uncertainties < 1MeV

The Ab Initio Mass Frontier: Tin



- systematics of overbinding similar to Ca/Ni
- not converged with respect to 3N matrix element truncation:

$$e_1 + e_2 + e_3 \leq E_{3\max}$$

(e_{1,2,3} : SHO energy quantum numbers)

need technical improvements to go further

Next Steps

Reach of Ab Initio Methods





Equations-of-Motion for Excitations



• describe "excited states" based on reference state:

$$\left|\Psi_{k}\right
angle\equiv R_{k}\left|\Psi_{0}
ight
angle$$

• (MR-)IM-SRG effective Hamiltonian in EOM approach:

$$[H(\infty), R_k] = \omega_k R_k, \quad \omega_k = E_k - E_0$$

- computational effort scales polynomially, vs. factorial scaling of Shell Model
- can exploit Multi-Reference capabilities (commutator formulation identical to flow equations)

complementary to Shell Model



• particle-hole excitations (TDA, RPA, Second RPA, ...)

$$R_{k} = \sum_{ph} R_{ph}^{(k)} : a_{p}^{\dagger} a_{h} : + \sum_{pp'hh'} R_{pp'hh'}^{(k)} : a_{p}^{\dagger} a_{p'}^{\dagger} a_{h'} a_{h} : + \dots$$

giant resonances

• particle attachment (analogous for removal):

$$R_{k} = \sum_{ph} R_{p}^{(k)} : a_{p}^{\dagger} : + \sum_{pp'h} R_{pp'h}^{(k)} : a_{p}^{\dagger} a_{p'}^{\dagger} a_{h} : + \dots$$

ground and excited states in odd nuclei

Effective Operators





- small radii: interaction issue (power counting, regulators, LECs, ...), also consider currents?
- implementation of electromagnetic & weak transition operators in progress; aim for consistent treatment: chiral EFT, SRG, IM-SRG (& Shell Model code !)

Magnus Series Formulation



• construct unitary transformation explicitly:

$$U(\mathbf{s}) = S \exp \int_0^{\mathbf{s}} d\mathbf{s}' \eta(\mathbf{s}') \equiv \exp \Omega(\mathbf{s})$$

• flow equation for Magnus operator :

$$\frac{d}{ds}\Omega = \sum_{k=0}^{\infty} \frac{B_k}{k!} \operatorname{ad}_{\Omega}^k(\eta) , \quad \operatorname{ad}_{\Omega}(O) = [\Omega, O]$$

(B_k: Bernoulli numbers)

- construct $O(s) = U(s)O_0U^{\dagger}(s)$ using Baker-Campbell-Hausdorff expansion (Hamiltonian + effective operators)
- generate systematic approximations to (MR-)IM-SRG(3)
- simple integrator sufficient (Euler!) unitarity built in

Example: Homogenous Electron Gas

S

G



Conclusions

Conclusions



- IM-SRG is a powerful *ab initio* framework for closed- and open-shell, medium-mass & (heavy) nuclei
- derivation of Shell-Model interactions (see talk by J. Holt)
 - immediate access to spectra, odd nuclei, intrinsic deformation (at Shell Model numerical cost)
- in progress:
 - EOM for odd nuclei and excited states
 - effective transition operators
 - approximate IM-SRG(3)
- new perspectives for old (?) problems: evolution of longrange correlations, construction of density functionals...

Acknowledgments



S. Bogner, T. Morris, Than Parzuchowski, F. Yuan Thank, Michigan State University orators: R. Furnstahl, S. König, S. More, R. Perry The Ohio State University

R. E. Gebrerufael, K. Hebeler R. Roth, A. Schwenk, J. Simonis, A. Gunther, Steinhardt, BS / Rare isotope Science Project, South Korea

S. Binder A. Cabiei, J. Langhammer T. Duguet, V. Somà Institut für Kernphysik, TU Darmstadt A. Calci, J. D. Holt, R. Stroberg

S. Bogner

NSCE, Binder, K. Wendt UT Knoxville & Oak Ridge National Laboratory

G. Papadimitriou

Iowa State University



Supplements

Scales of the Strong Interaction





quarks, gluons

chiral phase transition (de)confinement phase transition



Weinberg's 3rd Law of Progress in **Theoretical Physics:**

"You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"

momentum transfer (re:

Scales of the Strong Interaction





SRG in Two-Body Space

matrix elements

momentum space



 (\mathfrak{S})

G

Induced Interactions



- SRG is a unitary transformation in A-body space
- up to A-body interactions are induced during the flow:

$$\frac{dH}{d\lambda} = \left[\left[\sum a^{\dagger}a, \sum \underbrace{a^{\dagger}a^{\dagger}aa}_{2\text{-body}} \right], \sum \underbrace{a^{\dagger}a^{\dagger}aa}_{2\text{-body}} \right] = \dots + \sum \underbrace{a^{\dagger}a^{\dagger}a^{\dagger}aaa}_{3\text{-body}} + \dots$$

- state-of-the-art: evolve in three-body space, truncate induced four- and higher many-body forces (Jurgenson, Furnstahl, Navratil, PRL 103, 082501; Hebeler, PRC 85, 021002; Wendt, PRC 87, 061001)
- λ-dependence of eigenvalues is a diagnostic for size of omitted induced interactions

In-Medium SRG Flow: Diagrams





In-Medium SRG Flow: Diagrams





Results: Closed-Shell Nuclei





Phys. Rev. C 87, 034307 (2013), arXiv: 1212.1190 [nucl-th]

Variation of Scales





- variation of initial 3N cutoff only
- diagnostics for chiral interactions
- dripline at A=24 is robust under variations
- (leading) continuum effects too small to bind
 ²⁶O

H. Hergert - ESNT Workshop "Near-Degenerate Systems in Nuclear Structure and Quantum Chemistry from Ab Initio Methods", CEA Saclay, 03/31/2015