MSU Year 5 Status Report

I) Density Matrix Expansion/ab-initio EDFs

Scott Bogner
Juan Burgos (student)

II) In-medium SRG

Scott Bogner
Heiko Hergert
Koshiroh Tsukiyama**
Achim Schwenk**

**External

see M. Kortelainen’s talk
Year 5 in-medium SRG deliverables

• IM-SRG calculations of closed shell nuclei
  – modified truncation to treat “bare” interactions (N3LO)
  – alternative generators implemented
  – verified COM factorization using method of Hagen et al.
  – external HO trap implemented (closed shell neutron drops)

• Use in-medium SRG to develop valence shell model Hamiltonians and effective operators
  – Formalism developed and implemented for valence $H_{\text{eff}}$
  – Proof of principle calculations for $^6\text{Li}$ with K. Tsukiyama (Tokyo) and A. Schwenk (Darmstadt) completed.

• IM-SRG for infinite matter
  – include particle-hole channels (not there yet)
Year 5 papers with UNEDF support

1. “Testing the density matrix expansion against ab initio calculations of trapped neutron drops”
   S. K. Bogner, R. J. Furnstahl, H. Hergert, M. Kortelainen, P. Maris, M. Stoitsov and J. P. Vary

2. “Improved nuclear matter calculations from chiral low-momentum interactions”
   K. Hebeler, S. K. Bogner, R. J. Furnstahl, A. Nogga and A. Schwenk

3. “Microscopically-based energy density functionals for nuclei using the density matrix expansion: Implementation and pre-optimization”
   M. Stoitsov, M. Kortelainen, S. K. Bogner, T. Duguet, R. J. Furnstahl, B. Gebremariam and N. Schunck

4. “Operator Evolution via the Similarity Renormalization Group I: The Deuteron”

5. “In-Medium Similarity Renormalization Group for Nuclei”
   K. Tsukiyama, S. K. Bogner and A. Schwenk
   arXiv:1006.3639 [nucl-th] SPIRES entry (accepted to PRL)

6. “Microscopically-constrained Fock energy density functionals from chiral effective field theory. I. Two-nucleon interactions”
   B. Gebremariam, S. K. Bogner and T. Duguet
The Similarity Renormalization Group

Unitary transformation via flow equations:

$$\frac{dH_\lambda}{d\lambda} = [\eta(\lambda), H_\lambda] \quad \text{with} \quad \eta(\lambda) \equiv \frac{dU(\lambda)}{d\lambda} U^\dagger(\lambda)$$

Engineer $\eta$ to do different things as $\lambda \Rightarrow 0$

$$\eta(\lambda) = [\mathcal{G}_\lambda, H_\lambda]$$

$\mathcal{G}_\lambda = T \Rightarrow H_\lambda$ driven towards diagonal in $k$ – space

Rule of thumb: Take $\mathcal{G}_\lambda = H_\lambda^D$ where $H_\lambda = H_\lambda^D + H_\lambda^{OD}$

challenge: How to control induced many-body operators?
Normal Ordered Hamiltonians

\[ H = \sum t_i a_i^+ a_i + \frac{1}{4} \sum V_{ijkl}^{(2)} a_i^+ a_j^+ a_l a_k + \frac{1}{36} \sum V_{ijklmn}^{(3)} a_i^+ a_j^+ a_k a_n a_m a_l \]

Normal-order w.r.t. some reference state \( \Phi \) (e.g., HF):

\[ H = E_{vac} + \sum f_i N(a_i^+ a_i) + \frac{1}{4} \sum \Gamma_{ijkl} N(a_i^+ a_j^+ a_l a_k) + \frac{1}{36} \sum W_{ijklmn} N(a_i^+ a_j^+ a_k a_n a_m a_l) \]

\[ E_{vac} = \langle \Phi | H | \Phi \rangle \]

\[ f_i = t_{ii} + \sum_h \langle ih | V_2 | ih \rangle n_h + \frac{1}{2} \sum_{hh'} \langle ihh' | V_3 | ihh' \rangle n_h n_{h'} \]

\[ \Gamma_{ijkl} = \langle ij | V_2 | kl \rangle + \sum_h \langle ijh | V_3 | klh \rangle n_h \]

\[ W_{ijklmn} = \langle ijk | V_3 | lmn \rangle \]

\[ \langle \Phi | N(\cdots) | \Phi \rangle = 0 \]

0-, 1-, 2-body terms contain some 3NF effects thru density dependence => Efficient truncation scheme for evolution of 3N?
In-medium SRG for closed-shell nuclei (g.s.)

\[ H = \begin{array}{cccc}
0p0h & 1p1h & 2p2h & \ldots \\
\end{array} \]

Df. “offdiagonal” part of \( H \) as terms that mix \( 0p0h \) with higher \( ph \) sectors

\[ \eta(s) = [H(s), H^{\text{od}}(s)] \]

\[ \Gamma^{\text{od}} = \sum_{pp'h'hh'} \Gamma_{pp'h'h'} N(a_p^{\dagger}a_{p'}^{\dagger}a_ha_{h'}) + h.c \]

\[ f^{\text{od}} = \sum_{ph} f_{ph} N(a_p^{\dagger}a_h) + h.c. \]
In-medium SRG for closed-shell nuclei (g.s.)

\[
H(\infty) =  
\begin{array}{cccc}
0p0h & 1p1h & 2p2h & \cdots \\
\text{dark color} & & & \\
\end{array}
\]

HF reference state decouples from higher npnh states

\[
\lim_{s \to \infty} \langle \phi | H(s) | \phi \rangle = E_{gs}
\]

\[
QH(\infty)P = 0, \quad PH(\infty)Q = 0,
\]

where \( P = |\Phi\rangle \langle \Phi| \) and \( Q = 1 - P \).
$H^{\text{od}}$ gets suppressed.

Many-body methods w/evolved $H(s)$

MBPT converges more quickly

S-independent CCSD(T)

$\Rightarrow$ IM-SRG(2) is controllable approximation.

$\lambda \equiv s^{-1/4}$
Diagonalization of closed-shell systems

Initial results very good (soft interactions)

BUT

Much worse for harder interactions (e.g., N3LO)
Perturbative analysis of the IM-SRG

Important tool for
• the systematic organization of the flow equation
• the understanding of the relation to shell-model $H_{\text{eff}}/O_{\text{eff}}$

$$H(s) = H^{[0]}(s) + gH^{[1]}(s) + g^2H^{[2]}(s) + g^3H^{[3]}(s) + \cdots$$

$$\dot{H}^{[i]}(s) = \beta^{[i]}(H, s) \quad i = 0, 1, \cdots$$

Truncations based on n-body normal-ordered operators

<table>
<thead>
<tr>
<th></th>
<th>$E_{gs}$</th>
<th>SM $V_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>IM-SRG(2)</td>
<td>3rd-order exact</td>
<td>2nd-order exact</td>
</tr>
<tr>
<td>IM-SRG(3)</td>
<td>4th-order exact</td>
<td>3rd-order exact</td>
</tr>
</tbody>
</table>
Flow equation by perturbative analysis

Organization in terms of the power of g

\[
\dot{E}_0(s) = \eta^{(2)} \Gamma + \eta^{(1)} f + \eta^{(3)} W
\]

\[
\dot{\Gamma}(s) = \eta^{(2)} f + \eta^{(1)} \Gamma + \eta^{(2)} W + \eta^{(3)} \Gamma
\]

\[
\dot{W}(s) = \eta^{(3)} f + \eta^{(2)} W + \eta^{(3)} \Gamma
\]

- Truncation to 2-body N-ordered operators (terms in gray)
- Triples corrections to \( E_0 \) generated by 1- and 2-body terms in red
- Same corrections (sometimes w/opposite signs) generated by \( W, \eta^{(3)} \) terms omitted in 2-body N-ordered truncation. Dangerous for harder interactions!
Flow equation by perturbative analysis

Organization in terms of the power of g.

\[ \dot{E}_0(s) = [\eta^{(2)}, \Gamma][2] + [\eta^{(1)}, f][4] + [\eta^{(3)}, W][4] \]

\[ \dot{f}(s) = [\eta^{(1)}, f][2] + [\eta^{(2)}, \Gamma][2] + [\eta^{(3)}, f][3] + [\eta^{(2)}, W][3] + [\eta^{(3)}, \Gamma][3] + [\eta^{(3)}, W][4] \]

\[ \dot{\Gamma}(s) = [\eta^{(2)}, f][1] + [\eta^{(2)}, \Gamma][2] + [\eta^{(1)}, \Gamma][3] + [\eta^{(2)}, W][3] + [\eta^{(3)}, \Gamma][3] \]


For consistency, exclude 0-, 1-, 2-body terms in blue and red (IM-SRG(2)"

OR

include them along with 3-body terms (\eta^{(3)} and W)
Flow equation by perturbative analysis

Organization in terms of the power of $g$.

\[
\dot{E}_0(s) = \left[ \eta^{(2)}, \Gamma \right][2] + \left[ \eta^{(1)}, f \right][4] + \left[ \eta^{(3)}, W \right][4]
\]

\[
\dot{f}(s) = \left[ \eta^{(1)}, f \right][2] + \left[ \eta^{(2)}, \Gamma \right][2] + \left[ \eta^{(1)}, \Gamma \right][3] + \left[ \eta^{(2)}, f \right][3] + \left[ \eta^{(2)}, W \right][3] + \left[ \eta^{(3)}, \Gamma \right][3] + \left[ \eta^{(3)}, W \right][4]
\]

\[
\dot{\Gamma}(s) = \left[ \eta^{(2)}, f \right][1] + \left[ \eta^{(2)}, \Gamma \right][2] + \left[ \eta^{(1)}, \Gamma \right][3] + \left[ \eta^{(2)}, W \right][3] + \left[ \eta^{(3)}, \Gamma \right][3] + \left[ \eta^{(1)}, W \right][4] + \left[ \eta^{(3)}, f \right][4] + \left[ \eta^{(3)}, W \right][4]
\]

\[
\dot{W}(s) = \left[ \eta^{(3)}, f \right][2] + \left[ \eta^{(2)}, \Gamma \right][2] + \left[ \eta^{(2)}, W \right][3] + \left[ \eta^{(3)}, \Gamma \right][3] + \left[ \eta^{(1)}, W \right][4] + \left[ \eta^{(3)}, f \right][4]
\]

For consistency, exclude 0-, 1-, 2-body terms in blue and red (IM-SRG(2)')

OR

include them along with 3-body terms ($\eta^{(3)}$ and $W$)

IM-SRG(2)'

IM-SRG(2)
\( ^4 \)He with two different generators

\[
\eta^I = [H_D, H_{OD}] \quad \eta^I_{ij} = \frac{\langle i|H_{od}|j \rangle}{E_i - E_j}
\]
$^4$He with two different generators

Weak generator dependence

IM-SRG(2) and IM-SRG(2)' almost the same
Dependence on truncation for harder interactions

Consistent IM-SRG(2)’ truncation (solid) converges to CCSD result.

Substantial overbinding in each emax space for naive original IM-SRG(2) truncation (open).

**4He, N^3LO, \eta^H**
Generator dependence versus hw

\(\Delta E = E^I - E^0\) [MeV]

\(\hbar \omega\) [MeV]

- IM-SRG (green dashed line)
- IM-SRG' (green solid line)

**Strong generator and hw dependence**

**Weak generator and hw dependence**

IM-SRG(2)' truncation gives smaller generator dependence (~ basis independent)
Non-perturbative feature

Generator II
bare N3LO

\(^4\)He

\(\Lambda\text{-CCSD(T)}\)

\(\text{MBPT}(2)\) in \(\epsilon_{\text{max}} = 8\)

\(\text{MBPT}(3)\) in \(\epsilon_{\text{max}} = 8\)

- Agrees well with CCSD
- MBPT(2,3) breaks down
$^{16}$O with a hard NN interaction

- the IM-SRG(2)' gets closer to CCSD.
- works well for harder NN interactions.
$^{16}$O with a hard NN interaction

- small dependence on generator
- agrees w/CC theories for each model space
Evolution of operators

simultaneous evolution

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

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

\[
O_r(s) = O_r^{(0)}(s) + O_r^{(1)}(s) + O_r^{(2)}(s) \cdots
\]

RMS radius

\[
O_r(0) \equiv \frac{1}{A} \sum_i (\vec{r}_i - \vec{R}_{cm})^2
\]

\[
\langle r \rangle = \sqrt{\langle \psi | O_r(0) | \psi \rangle} = \lim_{s \to \infty} O_r^{(0)}(s)
\]
Radius of $^4$He

$$\frac{d}{ds} \mathcal{O}_r(s) = [\eta, \mathcal{O}_r(s)] \text{ with } \mathcal{O}_r \equiv \frac{1}{A} \sum_i (\vec{r}_i - \vec{R}_{cm})^2$$

charge radii by NCSM, similar trends

SKB et al., NPA801, 21 (2008)
Radii of $^{16}$O

$^{16}$O, N$^3$LO

$^{16}$O, Vsrg ($\lambda = 3.0$ fm$^{-1}$)

$^{16}$O, Vsrg ($\lambda = 2.5$ fm$^{-1}$)

$^{16}$O, Vsrg ($\lambda = 2.0$ fm$^{-1}$)
Shell model effective interactions from the IM-SRG

Passive valence orbitals \( \{q_i\} \)

Active valence orbitals \( \{v_i\} \)

hole orbitals \( \{h_i\} \)
Shell model effective interactions from the IM-SRG

Passive valence orbitals \( \{ q_i \} \)

Active valence orbitals \( \{ v_i \} \)

hole orbitals \( \{ h_i \} \)

\[
\begin{align*}
 f^{od}(s) &= \sum_{ph} f_{ph}(s) \{ a_p^\dagger a_h \} + \sum_{vq} f_{vq}(s) \{ a_v^\dagger a_q \} + \sum_{vh} f_{vq}(s) \{ a_v^\dagger a_h \} \\
 \Gamma^{od}(s) &= \sum_{pp'h'h'} \Gamma_{pp'h'h'}(s) \{ a_p^\dagger a_p'^\dagger a_h'a_h \} + \sum_{pp'vh} \Gamma_{pp'vh} \{ a_v^\dagger a_v'^\dagger a_h a_p \} \\
 &\quad + \sum_{vv'qq'} \Gamma_{vv'qq'}(s) \{ a_v^\dagger a_v'^\dagger a_q a_q \} + \sum_{vv'v''q} \Gamma_{vv'v''q} \{ a_v^\dagger a_v'^\dagger a_q a_q' \}
\end{align*}
\]
Details for valence shell model generators

“offdiagonal” terms $H_{OD}$ we want to drive to zero:

all operators that don’t annihilate valence model space vectors

AND

that change the number of valence shell excitations

$$\eta = [H_{OD}, H] \implies H(\infty) = E_0(\infty) + \hat{f}(\infty) + \hat{\Gamma}(\infty)$$

core g.s.  SM $H_{\text{eff}}$
Excitation spectra of $^6$Li versus NCSM result

$^6$Li, $V_{srg}$ ($\lambda=2.0$ fm$^{-1}$) $\hbar\omega = 20$ MeV
Excitation spectra of $^6$Li versus MBPT result

$^6$Li, $V_{sr}$ (λ=2.0 fm$^{-1}$)

$E_{\text{max}} = 8$

$1^+$

$2^+$

$0^+$

$3^+$

$1^+$

$Q^{(1)}$  $Q^{(2)}$  $Q^{(3)}$  IM-SRG  EXP

$E_x$ [MeV]
Excitation spectra of $^6\text{Li}$ versus MBPT + FD result
Summary and Outlook

- IM-SRG for closed-shell nuclei
  - implemented other generators
  - consistent truncation worked out based on MBPT content
  - harder interactions ("bare" n3lo) treated
  - Contamination of center of mass excitation is very small.
  - comparable to CCSD in current truncation
  - tools in place for benchmark paper of medium-mass nuclei (w/CC, SCGF, UMOA)

- Shell-model effective interactions for valence nucleons.
  - proof of principle for 6Li carried out
  - seems to outperform traditional MBPT methods
Summary and Outlook

Work in Progress

- initial 3N (normal ordered 0,1,2-body parts)
- **effective operator/Hamiltonian** for open-shell systems.
  - Effective interaction for valence shell nucleons (p, sd, fp).
  - Effective charge $\Rightarrow$ B(E2) for C, Ca, Ni and Sn.
  - Quenching factor for GT transition.
- Systematic improvement; 3-body flow equations (derived, not yet coded).
- particle-hole channels in infinite matter (H. Hergert)
- HFB reference state (H. Hergert)
Backups
Center of mass problem

Typical to nuclei = **self-bound** system, NO trapping fields

In the full Hilbert space

\[
[H_{\text{in}}, H_{\text{cm}}] = 0 \quad \Rightarrow \quad |\psi_A\rangle = |\psi_{\text{in}}\rangle \otimes |\psi_{\text{cm}}\rangle
\]

In a truncated space

\[
P(H_{\text{in}} + H_{\text{cm}})P |\psi_A\rangle = EP |\psi_A\rangle
\]

The condition for the decoupling of the w.f

\[
[PH_{\text{in}}P, PH_{\text{cm}}P] = 0 \iff [P, H_{\text{cm}}] = 0
\]

depends on the choice of P

Strategies to satisfy \([P, H_{\text{cm}}]=0\).

Use of HO function

- Jacobi coordinate
- Truncate the model space by the total HO excitations \(N_{\text{max}}\).

CM decoupling cannot be guaranteed for General many-body methods
Prescription for the IM-SRG

IM-SRG: truncation by the single-particle energy cutoff $e_{\text{max}}$. Generally $[P, H_{\text{cm}}] \neq 0$, the factorization of the w.f is unknown.

Assume that $H_{\text{cm}}$ is written by HO potential with c.m. coordinate, $R$ and $P$

$$H_{\text{cm}}(\tilde{\omega}) = \frac{P^2}{2mA} + \frac{1}{2}mA\tilde{\omega}^2 R^2 - \frac{3}{2}\hbar\tilde{\omega}$$

Evaluate $E_{\text{cm}}(\omega) = \langle H_{\text{cm}}(\omega) \rangle$ by evolving $H_{\text{cm}}(\omega)$

Estimate the optimal frequency for $H_{\text{cm}}(\tilde{\omega})$ following

$$\hbar\tilde{\omega} = \hbar\omega + \frac{2}{3}E_{\text{cm}}(\omega) \pm \sqrt{\frac{4}{9}E^2_{\text{cm}}(\omega) + \frac{4}{3}\hbar\omega E_{\text{cm}}(\omega)}$$
large $E_{cm}(\omega)$ when $\omega = \tilde{\omega}$

\[
\hbar \tilde{\omega} = \hbar \omega + \frac{2}{3} E_{cm}(\omega) \pm \sqrt{\frac{4}{9} E_{cm}^2(\omega) + \frac{4}{3} \hbar \omega E_{cm}(\omega)}
\]

almost constant $\hbar \tilde{\omega}$

small $E_{cm}(\tilde{\omega})$

4He, $V_{\text{SRG}}(\lambda=2.00\text{fm}^{-1})$, 7 shells
For $^{16}$O

almost constant $\hbar \tilde{\omega}$

$E_{\text{cm}}(\tilde{\omega}) / \hbar \tilde{\omega} \sim 1\%$

comparable to CC ($\sim 5\%$)
Perturbative solution of the IM-SRG(3)

The 2nd-order one-body term

\[
f_{ij}^{[2]}(s) = \frac{1}{2} e^{-\Delta_{ij}^2 s} \sum_{abc} (\bar{n}_a \bar{n}_b n_c + n_a n_b \bar{n}_c) V_{ciab} V_{abcj} \]

\[
\cdot \left[ \Delta_{ij} s (-\delta_{ciab} + \delta_{cjab}) + \frac{\bar{\delta}_{ciab} \bar{\delta}_{cjab}}{2} \left( \frac{1}{\Delta_{ciab}} + \frac{1}{\Delta_{cjab}} \right) (1 - e^{-2\Delta_{ciab} \Delta_{cjab} s}) \right]
\]

off-diagonal terms suppressed as \(e^{-2\Delta_{ij}^2 s}\)

\[
\delta_X := \begin{cases} 1 & \text{if } \Delta_X = 0 \\ 0 & \text{others} \end{cases} \quad \text{and} \quad \bar{\delta}_X = 1 - \delta_X
\]

\[
\lim_{s \to \infty} f_{ij}^{[2]}(s) = \begin{cases} 0 & (\varepsilon_i \neq \varepsilon_j) \\ \frac{1}{2} \sum_{abc; \Delta_{ciab} \neq 0} (n_a \bar{n}_b n_c + n_a n_b \bar{n}_c) \frac{V_{ciab} V_{abcj}}{\Delta_{ciab}} & (\varepsilon_i = \varepsilon_j) \end{cases}
\]

- Reproducing the Q-box (2nd order)
- Avoiding divergence of Fermion propagetors
- Possible for non-degenerate model space

\(\Rightarrow\) can be powerful alternative for Q-box expansion.
Perturbative solution of the IM-SRG(3)

A 3rd-order one-body term

\[ f_{ij}^{[3]}(\infty) \leftarrow \sum_{abcdx;\Delta \neq 0} \bar{n}_a \bar{n}_b n_c n_d \bar{n}_x \frac{V_{axdj} V_{bicx} V_{cdba}}{\Delta_{diax} \Delta_{cdab}} \]

\[ - \sum_{abcdx;\Delta \neq 0} \bar{n}_a \bar{n}_b n_c n_d \bar{n}_x \delta_{xaid} \frac{V_{axdj} V_{bicx} V_{cdba}}{\Delta_{cxbi} \Delta_{cdab}} \]

\[ \cdot \text{correction terms:} \]
\[ \cdot \text{disappear for the degenerate perturbation theory.} \]

\[ \cdot \text{automatically avoiding divergence due to zero denominator} \]
\[ \cdot \text{no need for the degenerate model space} \]
\[ \Rightarrow \text{can be powerful alternative for Q-box expansion.} \]

This holds for all the other terms in the 3rd order.
Error estimation

\[ \frac{d}{ds} \mathcal{O}_r(s) = [\eta, \mathcal{O}_r(s)] \text{ with } \mathcal{O}_r \equiv \frac{1}{A} \sum_i (\vec{r}_i - \vec{R}_{cm})^2 \]

\[
\mathcal{O}_r(0) = \left( \frac{1}{A} - \frac{1}{A^2} \right) \sum_{i=1}^{A} r_i^2 - \frac{1}{A^2} \sum_{i<j} A^2 r_i \cdot r_j (\equiv \mathcal{O}_r^I) \]
\[
= \frac{1}{A^2} \sum_{i<j} (\vec{r}_i - \vec{r}_j)^2 (\equiv \mathcal{O}_r^{II})
\]

Different initial conditions for SODE
In-medium SRG for Nuclear matter

- Normal order $H$ w.r.t. non-int. fermi sea
- Choose SRG generator to eliminate “off-diagonal” pieces

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

$$\eta = [\hat{f}, \hat{\Gamma}]$$

$$\lim_{s \to \infty} \Gamma_{od}(s) = 0$$

$$\langle 12 | \Gamma_{od} | 34 \rangle = 0 \text{ if } f_{12} = f_{34}$$

- Truncate to 2-body normal-ordered operators “IM-SRG(2)”
  - dominant parts of induced many-body forces included implicitly

$$H(\infty) = E_{\text{vac}}(\infty) + \sum f_i(\infty) N(a_i^\dagger a_i) + \frac{1}{4} \sum [\Gamma_d(\infty)]_{ijkl} N(a_i^\dagger a_j^\dagger a_l a_k)$$

$$E_{\text{vac}}(\infty) \rightarrow E_{gs}$$

$$f_k(\infty) \rightarrow \epsilon_k \text{ (fully dressed s.p.e.)}$$

$$\Gamma_d(\infty) \rightarrow f(k', k) \text{ (Landau q.p. interaction)}$$

Microscopic realization of SM ideas: dominant MF + weak A-dependent NN$_{\text{eff}}$
Correlations “adiabatically” summed into $H(\lambda)$

$\lambda \ [\text{fm}^{-1}]$

$E/A \ [\text{MeV}]$

$E_0$

$E_{\text{BHF}}$ (in-medium SRG)

$E_{\text{BHF}}$ (free-space SRG)

PNM*

Weak cutoff dependence over large range $\Rightarrow$ dominant $3,4,\ldots$-body terms evolved implicitly

*Neglects ph-channel. See Heiko Hergert’s talk.