In-medium Similarity Renormalization Group for nuclear many-body systems

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HPCI project “Large-scale quantum many-body calculations for nuclear property and it’s application”

In collaboration with
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Description of nuclei from NN/NNN

Methods should be controlled and improvable

Medium-mass nuclei

Light nuclei

Density functional theory
- Systematic
- computationally efficient
- Universal EDF unknown

$H_{\text{eff}}^{(v)} \Psi^{(v)} = (E - E_c) \Psi^{(v)}$

shell evolution, deformation, double-beta decay, ...

$ab\ initio\ H\Psi = E\Psi$

binding energy, radius
accuracy, feasibility
\[ H(\Lambda) = T_{\text{rel}} + V_{2N}(\Lambda) + V_{3N}(\Lambda) + V_{4N}(\Lambda) + \cdots \]

\[ \chi_{\text{EFT}} \]

- pion-exchange and short-range contact
- power counting (still open)
- systematic expansion
- many-body forces automatically

\[ V(k, k') \]

Low-momentum interactions

\[ V_{\text{low-k}, \text{SRG}} \]

Bogner-Schwenk-Furnstahl, PPNP, 65, 94 (2010)
Similarity Renormalization Group


The unitary evolution of the Hamiltonian via flow equation

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

\[ \eta(s) = \frac{dU(s)}{ds} U^\dagger(s) \]

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

by F. Wegner

\[ \frac{d}{ds} \text{Tr} \left\{ (H^{od})^2 \right\} \leq 0 \]

Flexibility of choosing the \( H^d(s) \) for a particular problem.

cutoff \( \lambda \equiv s^{-1/4} \) as evolution variable

\[ H^d(s) = T \]

Bogner et al, PRC75, 061001(R) (2007)

\[ H^d(s) = \begin{pmatrix} PH(s)P & 0 \\ 0 & QH(s)Q \end{pmatrix} \]

Anderson et al, PRC77, 037001 (2008)
RG and many-body interactions

Free-space SRG, evolving consistent 3N interactions => exact method

- NN only => $\lambda$-dependent
- + induced NNN => almost $\lambda$-independent

Jurgenson, Furnstahl and Navratil, PRL103, 082501(2009)

same trend for heavier systems
Roth et al., PRL107, 07201(2011)

$$H(s) = U(s)H^{(2)}U^\dagger(s) = \tilde{H}^{(2)}(s) + \tilde{H}^{(3)}(s) + \cdots$$

In-medium SRG

- Defined in many-body system (finite density)
- Approximate evolution of 3-, .. A-body operators within 2b machinery.
- Different SRG evolutions for different mass regions.

Normal-ordered Hamiltonian

\[ \hat{H} = \sum_{ij} T_{ij} a_i^\dagger a_j + \frac{1}{2!} \sum_{ijkl} V_{ijkl}^{(2)} a_i^\dagger a_j^\dagger a_l a_k + \frac{1}{3!} \sum_{ijklmn} V_{ijklmn}^{(3)} a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n + \cdots \]

Normal order w.r.t. a finite-density Fermi vacuum \(|\Phi\rangle\), e.g. HF.

\[ H = E_0 + \sum_{ij} f_{ij} \{ a_i^\dagger a_j \} + \frac{1}{2!} \sum_{ijkl} \Gamma_{ijkl} \{ a_i^\dagger a_j^\dagger a_l a_k \} + \frac{1}{3!} \sum_{ijklmn} W_{ijklmn} \{ a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n \} \]

where coefficients of normal-ordered operators are given by

\[ E_0 = \langle \Phi | H | \Phi \rangle = \sum_k T_{kk} n_k + \frac{1}{2} \sum_{ij} V_{ij}^{(2)} n_i n_j + \frac{1}{6} \sum_{ijk} V_{ijk}^{(3)} n_i n_j n_k \]

\[ f_{ij} = T_{ij} + \sum_k V_{ikj}^{(2)} n_k + \frac{1}{2} \sum_{kl} V_{ikl}^{(3)} n_k n_l \]

\[ \Gamma_{ijkl} = V_{ijkl}^{(2)} + \frac{1}{4} \sum_m V_{ijmkl}^{(3)} n_m \]

\[ W_{ijklmn} = V_{ijklmn}^{(3)} \]

3-body and higher-body interactions through density-dependent coefficients. => may be efficient truncation scheme
Decoupling (schematic picture)

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

\( \eta(s) \) is determined \( s \) as to eliminate \( H^{od}(s) \)

Decouples ground state

\[ H^{od} = f_{ph} + \Gamma_{pphh} \]

Vertices connecting reference state and \( np-nh \) excited states

Decouples valence space

\[ H^{od} = f_{ph} + \Gamma_{pphh} + f_{vq} + f_{vh} + \Gamma_{vv'qq'} + \Gamma_{vhpp'} + \Gamma_{vv'v''h} \]

Vertices connecting valence space and outside of it.
**In-medium SRG flow equation**

\[
\frac{dH(s)}{ds} = [\eta, H(s)] = [\eta^{(1)} + \eta^{(2)} + \eta^{(3)} + \cdots, f + \Gamma + W + \cdots]
\]

commutator form \(\Rightarrow\) no unlinked diagram

\(\Rightarrow\) size extensive: energy scales linearly w/ # of particles

**Flow eqns.**

\[
\frac{d}{ds} E_0(s) = 2 \sum_{ab} n_a \bar{n}_b \eta_{ab}^{(1)} f_{ba} + \frac{1}{2} \sum_{abcd} \eta_{abcd} \Gamma_{cdab}(s) n_a n_b \bar{n}_c \bar{n}_d
\]

\[
+ \frac{1}{18} \sum_{abcdef} \eta_{abcdef}^{(3)} W_{defabc} n_a n_b n_c \bar{n}_d \bar{n}_e \bar{n}_f
\]

\[
\frac{d}{ds} \Gamma_{ijkl}(s) = \sum_a \left\{ (1 - P_{ij}) (\eta_{ia}^{(1)} \Gamma_{ajkl} - f_{ia} \eta_{ajkl}^{(2)}) - (1 - P_{kl}) (\eta_{ai}^{(1)} \Gamma_{ijal} - f_{ai} \eta_{ijal}^{(2)}) \right\}
\]

\[
+ \frac{1}{2} \sum_{ab} (1 - n_a - n_b) (\eta_{ijab}^{(2)} \Gamma_{abkl} - \Gamma_{ijab} \eta_{abkl}^{(2)})
\]

\[- \sum_{ab} (n_a - n_b) \left[ (1 - P_{ij})(1 - P_{kl}) \eta_{bijal}^{(2)} \Gamma_{aibk} \right]
\]

\[
+ \sum_{ab} (n_a - n_b) \left( \eta_{aibkl}^{(3)} f_{ba} - W_{aibkl} \eta_{ba} \right)
\]

**IM-SRG(2):** \(n^6\), **IM-SRG(3):** \(n^8\)

\(\text{pp or hh}\) \(\text{ph}\)
Non-Perturbative feature: Schematic

The flow equation can essentially be seen as

\[ \Gamma[n+1] = \Gamma[n] + \text{[diagram]} + \text{[diagram]} \]

With the initial condition

\[ \Gamma[0] = \text{[diagram]} =: V(\text{bare two-body coupling}) \]
Non-Perturbativeness of IM-SRG: Schematic

Solving the flow equation step by step

Correlations to all order

\( \Gamma[1]= \)

\( \Gamma[2]= \)

\( V \)

\( \mathcal{O}(V^2) \)

\( \mathcal{O}(V^3) \)

\( \mathcal{O}(V^4) \)

...
Flow equation by perturbative analysis

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

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

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

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

- **IM-SRG(2):** 3rd-order exact for GS energy and 2nd-order exact for \(V_{\text{eff}}\).
- **IM-SRG(3):** 4th-order exact for GS energy and 3rd-order exact for \(V_{\text{eff}}\).
- **IM-SRG is controlled and improvable** method
Numerical calculations

\[ H(0) = T_{\text{rel}} + V_{NN} + V_{3N} + V_{4N} + \cdots \]

N\(^3\)LO (\(A=500\text{MeV}\)) from \(\chi\)EFT
Free-space SRG evolved version \(V_{\text{srg}}(\lambda)\)

Bogner-Perry-Furnstahl, PRC 75, 061001 (2008)

\[ \frac{d}{ds} f(s) = \beta(f, s) \]

\begin{tabular}{|c|c|c|}
\hline
\(e_{\text{max}}\) & \# SP & \(\text{dim}(f)\) \\
\hline
4 & 30 & \(3.4 \times 10^4\) \\
5 & 42 & \(1.5 \times 10^5\) \\
6 & 56 & \(4.7 \times 10^5\) \\
7 & 72 & \(1.4 \times 10^6\) \\
8 & 90 & \(3.5 \times 10^6\) \\
10 & 130 & \(2.0 \times 10^7\) \\
\hline
\end{tabular}
\( ^4\text{He} \) with two different generators

- Truncation up to normal-ordered 2-body level is a good approximation.
• Agrees well with CCSD (95% of correlation)
• MBPT(2,3) break down
• IM-SRG(2) work for $^{16}$O and $^{40}$Ca
$H^{\text{od}}$ gets suppressed.
Evolution of operators

Arbitrary operator evolved on equal footing

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

\[ \frac{d}{ds} O_r(s) = [\eta, O_r(s)] \quad O_r(s) = O_r^{(0)}(s) + O_r^{(1)}(s) + O_r^{(2)}(s) \ldots \]

E.g., RMS radius

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

\[ \langle r \rangle = \sqrt{\langle \psi | \hat{O}_r(0) | \psi \rangle} = \lim_{s \to \infty} \sqrt{O_r^{(0)}(s)} \]

Joint benchmark is ongoing (NCFC, IT-NCSM, CCM, MBGF, UMOA, IM-SRG)
Results agree within uncertainty

Next step from H. Kamada et al., PRC64:044001(2001)
Ground-state convergence in $^6\text{Li}$ ($^4\text{He}+\text{"2"}$ vs 6)

**Effective 2-body problem**

- $e_{\text{max}} = 4$
- $e_{\text{max}} = 6$
- $e_{\text{max}} = 8$
- $e_{\text{max}} = 10$

**6-body problem**

- $N_{\text{max}} = 2$
- $N_{\text{max}} = 4$
- $N_{\text{max}} = 6$
- $N_{\text{max}} = 8$
- $N_{\text{max}} = 10$

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**IM-SRG $H_{1}^{\text{od}}$**

- Ground-state energy vs $h\nu$ [MeV]

**IM-SRG $H_{2}^{\text{od}}$**

- Ground-state energy vs $h\nu$ [MeV]

**NCSM**

- Extrapolation

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**Plot Details**

- Line styles and markers indicate different values of $e_{\text{max}}$ and $N_{\text{max}}$.
The graph shows the comparison of IM-SRG and NCSM for the spectrum of the $^6$Li. The figure highlights the effective 2-body problem and the 6-body problem. The $^6$Li, Vsrg with $(\lambda = 2.0 \text{ fm}^{-1})$ and $\hbar \omega = 24 \text{ MeV}$ are plotted. The graph indicates that IM-SRG works for 18-body as well.
Summary

We introduced SRG evolution of Hamiltonian in many-body medium (IM-SRG).

We numerically demonstrated the features of in-medium SRG.

- Decoupling of a Hamiltonian, Size-extensivity, Non-perturbative feature.
- Radius (arbitrary operators can be evolved).
- Contamination of center of mass excitation is very small.
- Shell-model effective interactions for valence nucleons (p and sd).

Work in Progress

- Derivation of effective operator.
- Systematic improvement; 3-body flow equations.