In-medium similarity renormalization group for nuclei and nuclear matter

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Punch lines of my talk

The in-medium SRG (thru the magic of normal-ordering) suggests the following intriguing possibilities:

- RG evolution of 3-body (and higher) interactions with NN machinery
- Microscopic basis for phenomenological SM and Landau Fermi Liquid Theory
- new ab-initio method in and of itself?
“Resolution-Dependent” Sources of Non-perturbative Physics

- strong core repulsion
- strong tensor forces
- deuteron pole
- pairing instability

scheme-dependent, U.V. details
(e.g., resolution scale $\Lambda$)

scheme-independent
(physical, independent of UV details)

Strong coupling of low- and high-$k$ $\leftrightarrow$ Strong SRC’s
Renormalization methods to **decouple** high-k

- **Bloch-Horowitz**
  - simple (either “integral” or RGE form) ☺
  - energy-dependent (issues with size extensivity, c.f. Brandow et al.) ☹

- **Lee-Suzuki**
  - energy independent ☺
  - complicated “integral” or RGE form (need to diagonalize a-body problem for a-body $H_{\text{eff}}$) ☹

- **Similarity RG**
  - energy independent ☺
  - simple RGE form (**never** diagonalize a-body problem) ☻
The Similarity Renormalization Group  
[Wegner, Glazek and Wilson]

- Unitary transformation on an initial $H = T + V$
  $$H_s = U(s)HU\dagger(s) \equiv T + V_s \quad s = \text{continuous flow parameter}$$

- Differentiating with respect to $s$:
  $$\frac{dH_s}{ds} = [\eta(s), H_s] \quad \text{with} \quad \eta(s) \equiv \frac{dU(s)}{ds}U\dagger(s) = -\eta\dagger(s)$$

- Engineer $\eta(s)$ to do different things as $s \to \infty$
  $$\eta(s) = [G_s, H_s]$$

  $G_s = T \Rightarrow H_s \text{ driven towards the diagonal in } k - \text{space}$

  $G_s = PH_sP + QH_sQ \Rightarrow H_s \text{ driven towards block diagonal form}$

  \[\vdots\]
SRG evolved NN interactions with $\eta = [T, H]$

- In each partial wave with $\epsilon_k = \hbar^2 k^2 / M$ and $\lambda^2 = 1 / \sqrt{s}$

$$\frac{dV_\lambda}{d\lambda}(k, k') \propto - (\epsilon_k - \epsilon_{k'})^2 V_\lambda(k, k') + \sum_q (\epsilon_k + \epsilon_{k'} - 2\epsilon_q) V_\lambda(k, q) V_\lambda(q, k')$$

$^1S_0 \quad \lambda = 10.0 \text{ fm}^{-1}$

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In each partial wave with $\epsilon_k = \hbar^2 k^2 / M$ and $\lambda^2 = 1 / \sqrt{s}$

$$\frac{dV^\lambda_{\lambda}}{d\lambda}(k, k') \propto - (\epsilon_k - \epsilon_{k'})^2 V_{\lambda}(k, k') + \sum_q (\epsilon_k + \epsilon_{k'} - 2\epsilon_q) V_{\lambda}(k, q) V_{\lambda}(q, k')$$

$^1S_0$ \(\lambda = 3.0 \text{ fm}^{-1}\)

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$^1S_0 \quad \lambda = 2.0 \text{ fm}^{-1}$

$\lambda = 2.0 \text{ fm}^{-1}$
Flexibility of SRG methods

Can reproduce “conventional” Lee-Suzuki Block-Diagonalization

Key Difference: In SRG approach one never has to diagonalize a cluster problem.
Decoupling high-\(k\) and low-\(k\) \(\Rightarrow\) accelerated convergence, more perturbative

**BUT note...**

\(\lambda\)-dependent results (omitted induced 3...A-body forces)
SRG Evolution and Many-Body Forces

- Many-body interactions induced during the flow

\[
\frac{dV_s}{ds} = \left[ \sum a^\dagger a, \sum a^\dagger a^\dagger a a \right], \sum a^\dagger a^\dagger a a = \cdots + \sum a^\dagger a^\dagger a^\dagger a a a + \cdots
\]

In principle up to A-body operators generated

- Is this a problem?
  - Not if “induced” terms are of natural size
  - \(\lambda\)-dependence \(\Rightarrow\) tool to assess truncation errors
  - They’re there to begin with anyway. Might as well have them be soft and develop the SRG machinery to evolve them.
Recent developments in 3N SRG evolution

(Jurgenson, Furnstahl, Navratil)

It works! $\lambda$-independent $^3$H, softer convergence

Induced 4N are $\approx 0$ for $\lambda \geq 2 \text{ fm}^{-1}$...
Free space versus in-medium SRG

Free space SRG: \( V(\lambda)_{2N} \) fixed in 2N system
\[ V(\lambda)_{3N} \] fixed in 3N system
\[ \vdots \]
\[ V(\lambda)_{aN} \] fixed in aN system

Use \( T + V(\lambda)_{2N} + V(\lambda)_{3N} + \ldots + V(\lambda)_{aN} \) in A-body system

In-medium SRG: evolution done at finite density (i.e., directly in A-body system). Different mass regions ⇒ require different SRG evolutions

inconvenience outweighed (?) by simplifications allowed by normal-ordering
Normal Ordered Hamiltonians

Pick a reference state $\Phi$ (e.g., HF) and apply Wick’s theorem to 2nd-quantized Hamiltonian

\[ A_i A_j A_k A_l \cdots A_m = N(A_i A_j A_k A_l \cdots A_m) \]
\[ + N\left(\overline{A_i A_j A_k A_l \cdots A_m} + \text{all other single contractions}\right) \]
\[ + N\left(\overline{A_i A_j A_k A_l \cdots A_m} + \text{all other double contractions}\right) \]
\[ \vdots \]
\[ + N\left(\text{all fully contracted terms}\right) \]

\[ a_i^\dagger a_j = \delta_{ij} \theta(\epsilon_F - \epsilon_i) \quad a_i a_j^\dagger = \delta_{ij} \theta(\epsilon_i - \epsilon_F) \]

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

Exactly re-cast $H$ as:

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

$$
E_{vac} = \langle \Phi | H | \Phi \rangle
$$

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

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

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

0-, 1-, 2-body terms contain some 3NF effects thru density dependence => Efficient truncation scheme?
Normal Ordering Truncations

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

Good truncation for CC (closed shell) and making contact to phenomenological SM monopole corrections

(Hagen et al.)

Other operators? Resolution dependence of truncations? Open shell systems and multi-reference N-ordering?

Schwenk et al.
In-medium SRG for Infinite NM

- Normal order $H$ w.r.t. non-interacting fermi sea
- Choose SRG generator to eliminate "energy off-diagonal" pieces

$$\eta = [\hat{f} + \hat{\Gamma}_d, \hat{\Gamma}] = [\hat{f}, \hat{\Gamma}] + \mathcal{O}\left(\frac{1}{A}\right) \quad \Rightarrow \quad \lim_{s \to \infty} \Gamma_{od}(s) = 0$$

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

- Truncate flow equations to < 2-body normal-ordered operators
  - dominant parts of induced many-body forces included implicitly

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

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

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

$$\Gamma_d(\infty) \quad \rightarrow \quad f(k', k) \quad \text{(Landau q.p. interaction)}$$
In-medium SRG Equations Infinite Matter

0-body flow

\[ \frac{d}{ds} E_{\text{vac}} = \frac{1}{2} \sum_{ijkl} (f_{ij} - f_{kl}) |\langle ij | \Gamma | kl \rangle|^2 n_i n_j \bar{n}_k \bar{n}_l \]

1-body flow

\[ \frac{d}{ds} f_a = \sum_{bcd} (f_{ad} - f_{bc}) |\langle ad | \Gamma | bc \rangle|^2 (\bar{n}_b \bar{n}_c n_d + n_b n_c \bar{n}_d) \]

interference of 2p1h 2h1p self-energy terms
In-medium SRG Equations Infinite Matter

2-body flow

\[
\langle 12 | \frac{d\Gamma}{ds} | 34 \rangle = -(f_{12} - f_{34})^2 \langle 12 | \Gamma | 34 \rangle \\
+ \frac{1}{2} \sum_{ab} (f_{12} + f_{34} - 2f_{ab}) \langle 12 | \Gamma | ab \rangle \langle ab | \Gamma | 34 \rangle (1 - n_a - n_b) \\
+ \sum_{ab} [(f_{1a} - f_{3b}) - (f_{2b} - f_{4a})] \langle 1a | \Gamma | 3b \rangle \langle b2 | \Gamma | a4 \rangle (n_a - n_b) \\
- \sum_{ab} [(f_{2a} - f_{3b}) - (f_{1b} - f_{4a})] \langle 2a | \Gamma | 3b \rangle \langle b1 | \Gamma | a4 \rangle (n_a - n_b)
\]

Note the interference between s, t, u channels a-la Parquet theory
SRG is manifestly non-perturbative

\[ \Gamma(\delta s) \sim \]

\[
\begin{array}{cccc}
\quad & \quad & \quad & \quad \\
\quad & \quad & \quad & \quad \\
\quad & \quad & \quad & \quad \\
\quad & \quad & \quad & \quad \\
\end{array}
\]
SRG is manifestly non-perturbative

$\Gamma(\delta s) \sim \Gamma(2\delta s) \sim$
SRG is manifestly non-perturbative

\[ \Gamma(\delta s) \sim \]

\[ \Gamma(2\delta s) \sim \]

+ many more ...
Some observations

1) \( \frac{d}{ds} \langle H \rangle_0 \leq 0 \) for monotonic \( f_k \) correlations weakened, HF picks up more binding with increasing \( s \).

2) pp channel + 2 ph channels treated on equal footing

3) Functional derivatives to make contact with induced many-body forces in the original (not normal-ordered) representation

\[
\langle ijk \mid \frac{dV_3}{ds} \mid lmk \rangle = \frac{\delta}{\delta n_k} \left[ \langle ij \mid \frac{d\Gamma}{ds} \mid lm \rangle \right] \{n=0\}
\]

Etc…

4) no unlinked diagrams (size extensive, etc.)

5) Extension to effective operators immediate
Example: Perturbative content of SRG

- Solve SRG eqns to 2nd-order the bare coupling

\[
E_0(s) \approx E_0(0) + \frac{1}{4} \sum_{1234} n_1 n_2 \bar{n}_3 \bar{n}_4 \frac{|V_{1234}(0)|^2}{f_{12} - f_{34}} \left(1 - e^{-s(f_{12} - f_{34})^2}\right)
\]

\[
E_{\text{corr}}(s) \approx \frac{1}{4} \sum_{1234} n_1 n_2 \bar{n}_3 \bar{n}_4 \frac{|V_{1234}(0)|^2}{f_{12} - f_{34}} e^{-s(f_{12} - f_{34})^2}
\]

As s increases, contributions shuffled from correlation energy into
The non-interacting VEV contribution (I.e., Hartree-Fock)

Microscopic connection to shell model?
(MF + “weak” A-dependent residual NN interaction)
In-medium SRG in 1D nuclear matter

Free-space SRG evolution truncated at NN level

\[ E/A \]

\[ \lambda \]

1D Nuclear Matter at \( \rho_0 \)

- HF approaches ladder sum at lower \( \lambda \) (weak correlations)

\[ \text{BUT} \]

- Strong \( \lambda \)-dependence due to truncation to 2N SRG

\[ \text{try in-medium SRG w/ normal-ordering to reduce the } \lambda \text{-dependence} \]
In-medium SRG in 1D nuclear matter

In-medium SRG evolution truncated at normal-ordered NN level

- HF approaches ladder sum at lower $\lambda$ (weak correlations)

AND

- $\lambda$-dependence weak (dominant many-body forces kept by normal ordering).
In-medium SRG in Real 3D nuclear matter

In-medium SRG evolution truncated at normal-ordered NN level

• HF approaches ladder sum at lower $\lambda$ (weak correlations)

• $\lambda$-dependence weak (dominant many-body forces kept by normal ordering).

• Soon: ph-channel terms

* Neglected ph channel, angle-averaging, ...
In-medium SRG in Real 3D nuclear matter

In-medium SRG evolution truncated at normal-ordered NN level

- HF approaches ladder sum at lower $\lambda$ (weak correlations)
- $\lambda$-dependence weak (dominant many-body forces kept by normal ordering)
- Soon: ph-channel terms

Neglected ph channel, angle-averaging, ...
Application to nuclei (K. Tsukiyama, SB, A. Schwenk)

minor annoyance:  
\[ \hat{f} = \sum_i f_i N(a_i^\dagger a_i) \rightarrow \sum_{ij} f_{ij} N(a_i^\dagger a_j) \]

SRG generator:  
\[ \eta = [\hat{f}^d + \hat{\Gamma}^d, \hat{f}^{od} + \hat{\Gamma}^{od}] \]

\[ f_{ij}^d = 0 \quad (\epsilon_i \neq \epsilon_j) \quad \Gamma_{ijkl}^d = 0 \quad (\epsilon_i + \epsilon_j \neq \epsilon_k + \epsilon_l) \]

\[ \epsilon_i = \text{HO sp energy} \]
SRG flow of $E_{\text{vac}}$ for He-4

$p_{\text{lim}}$

$E_0(^4\text{He}) [\text{MeV}]$

$N_{\text{max}}=2$

$N_{\text{max}}=3$

$N_{\text{max}}=4$

$N_{\text{max}}=5$

NCSM = $-24.8 \text{MeV}$

0 0.5 1

$s [\text{MeV}^{-2}]$

In progress: perturbative corrections from non-zero $\Gamma$ in the block-diagonal structure

Alternative SRG generators using HF energies to define “diagonal” and “off-diagonal”

O16 and Ca40 next...
SRG flow of 1-body (s.p.e.’s)

One-body flow $g_{ij}(s)$ [MeV]

(not even) preliminary
Summary of In-Medium SRG w/Normal-Ordering

- 2N formalism includes dominant induced 3,...A-body forces
- Microscopically obtain dominant MF + “weak” residual interaction
- 1st 3D nuclear matter results look pretty good, still need ph terms
- Non-perturbative path to shell model $H_{\text{eff}}$ and $O_{\text{eff}}$?
- Ab-initio method to diagonalize medium nuclei?
- First applications to finite nuclei gearing up
- More sophisticated reference state to normal order w.r.t.?
  - quasiparticle vacuum (pairing)
  - multi-reference (open shell systems)