MSU Year 3 Status Report

Pt.1: In-medium SRG
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Pt.2: Density Matrix Expansion EDF from chiral NN and NNN interactions
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**External
MSU Year 3 Accomplishments

• **New development**: In-medium SRG
  – 1st tests in infinite matter and light closed shell nuclei

• DME for chiral EFT NN and NNN **completed**
  – analytic expressions for all couplings
  – codes available
  – fully automated (symbolic tools)
    • more complicated terms (N3LO NNN, NNNN, ...)

• Improved DME for vector part **completed**
  – parameter free
  – relative errors reduced by factor of 5-10

• Validation of DME against exact HF **in-progress**
  – role of self-consistency, exact Hartree
Normal Ordered Hamiltonians

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

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

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

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

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

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

\[ W_{ijklmn} = \langle ijk | V_3 | lmn \rangle \quad \langle \Phi | N(\cdots) | \Phi \rangle = 0 \]

0-, 1-, 2-body terms contain some 3NF effects thru density dependence \( \Rightarrow \) Efficient truncation scheme for evolution of 3N?
In-medium SRG for Infinite NM

• Normal order H w.r.t. fermi sea

• Choose SRG generator to eliminate “energy 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 flow equations to 2-body normal-ordered operators
  - dominant parts of induced many-body forces included implicitly

\[ H(\infty) = E_{vac}(\infty) + \sum f_i(\infty)N(a_i^\dagger a_i) + \frac{1}{4} \sum [\Gamma_d(\infty)]_{ijkl}N(a_i^\dagger a_j^\dagger a_l a_k) \]
\[ E_{vac}(\infty) \to E_{gs} \]
\[ f_k(\infty) \to \epsilon_k \text{ (fully dressed s.p.e.)} \]
\[ \Gamma_d(\infty) \to f(k', k) \text{ (Landau q.p. interaction)} \]

Microscopic realization of SM ideas: dominant MF + weak A-dependent NN_{eff}
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

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

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

2-body flow

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

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

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

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\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 ...
In-medium SRG in nuclear matter

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

Symmetric Nuclear Matter

\( k_F = 1.4 \text{ fm}^{-1} \)

\( N^3\text{LO}(500) \)

\[ \lambda \equiv s^{-1/4} \]

- HF approaches BHF at lower \( \lambda \) (weak correlations, mean field becomes exact)

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

* Neglected ph channel
**In-medium SRG in neutron matter**

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

- HF approaches BHF at lower $\lambda$ (weak correlations, mean field becomes exact)
- $\lambda$-dependence weak (dominant many-body forces kept by normal ordering).

* Neglected ph channel
In-medium SRG: rest of year 3 and year 4

- Infinite nuclear/neutron matter
  - inclusion of ph-channels
  - pairing (N-order w.r.t. BCS)

- Finite nuclei (Koshiroh Tsukiyama, SKB, A. Schwenk)
  - closed shell nuclei
  - non-perturbative calculations of valence SM $H_{\text{eff}}$ and $O_{\text{eff}}$
What’s missing in Skyrme?

• Density dependencies too simplistic (integer powers)
• Isovector components not well constrained (no pions)
• What’s the connection to many-body forces? E.g., spin-orbit too simplistic (at microscopic level NN is short-ranged while NNN is long-ranged)

Use DME to build missing finite range NN + NNN pion exchanges into Skyrme
Local EDFs from Many-Body Theory

• Dominant MBPT contributions take the form

\[ \langle V \rangle \sim Tr_1 Tr_2 \int dR \, dr_1 \, dr_2 \, dr_3 \, \rho(r_1, r_3) K(r_1, r_3) \rho(r_2, r_4) + \text{NNN} \cdots \]

• Density Matrix Expansion (Negele & Vautherin)

\[ \langle \Phi | \psi^\dagger(R - \frac{1}{2} r) \psi(R + \frac{1}{2} r) | \Phi \rangle = \sum_n \Pi_n(k_F r) \langle \mathcal{O}_n(R) \rangle \]

\[ \langle \mathcal{O}_n(R) \rangle = [\rho(R), \nabla^2 \rho(R), \tau(R), J(R), \ldots] \]

• Maps MBPT into a Skyrme-like EDF

\[ \langle V \rangle \sim \sum_{n,m} \int dR \, \mathcal{O}_n(R) \mathcal{O}_m(R) \int dr \, \Pi_n(k_F r) \Pi_m(k_F r) V_{2N}(r) + 3N \]

Finite range V \iff novel density dependent couplings
Including Long Range Chiral EFT in Skyrme–like EDFs

DME functional from chiral NN + NNN at HF level

\[ E[\rho] = \sum_q \int d\mathbf{R} \left\{ A^{\rho \rho} \rho_q^2 + A^{\rho \tau} \rho_q \tau_q + A^{\rho \Delta \rho} \rho_q \Delta \rho_q + A^{\nabla \rho \nabla \rho} \nabla \rho_q \nabla \rho_q + \cdots \right\} \]

Chiral EFT NN + NNN interactions

\[ V = V_{ct}(\Lambda) + V_{1\pi} + V_{2\pi} + \cdots \]

Each coupling function splits into 2 terms

1) Skyrme-like coupling constants from contact terms
2) \( \rho \)-dependent coupling functions from pion exchanges

\[ A^{\rho \tau} \Rightarrow A^{\rho \tau}(\Lambda) + A^{\rho \tau}[\rho] \]

DME at HF level still relevant since higher orders MBPT (G-matrices) “heal” at long-distances
Including Long Range Chiral EFT in Skyrme-like EDFs

- DME coupling functions from \textit{finite range} NN and NNN chiral EFT

- Refit Skyrme coupling constants (EFT constraints $\Rightarrow$ naturalness, $\Lambda$-dependence, etc.)

- Look for improved observables and for sensitivities
Nothing crazy with prelim. NM/surface refits... (Mario’s talk)

\[ C^{ijk}[u] \xi_i \xi_j \xi_k, \quad u \equiv \frac{k_F(R)}{m_\pi} \]

NOTE: No inclusion of N2LO NNN contributions
Long-range pion exchange contributions to the EDF

Longest range $V \iff$ Strongest density dependence in EDF

Novel density-dependencies in EDF from $1\pi$ and $2\pi$ exchanges:

$$\rho^{7/3}, \rho^{4/3}, \rho^{2/3}, \frac{1}{\rho^{2/3}} \log(1 + c\rho^{2/3}), \ldots$$
DME for chiral NNN force (N2LO)

- Expect interesting spin-orbit/tensor couplings from TPE

\[ V_c(q_1, q_2, q_3) \sim \frac{\sigma_1 \cdot q_1 \sigma_2 \cdot q_2}{(q_1^2 + m_\pi^2)(q_2^2 + m_\pi^2)} F^{\alpha\beta}_{123} \tau_1^{\alpha} \tau_2^{\beta} + \text{perms} \]

\[ F^{\alpha\beta}_{123} \equiv \delta_{\alpha\beta} \left[ -4 \frac{c_1 m_\pi^2}{f^2_\pi} + 2 \frac{c_3}{f^2_\pi} q_1 \cdot q_2 \right] + \frac{c_4}{f^2_\pi} \epsilon^{\alpha\beta\gamma} \tau_3^\gamma \sigma_3 \cdot (q_1 \times q_2) \]

- Complexity explodes (symbolic tools developed by B. Gebremariam)

\[
\langle V_{3N}^{\text{HF,dir}} \rangle = \frac{1}{2} \text{Tr}_1 \text{Tr}_2 \text{Tr}_3 \int d\bar{r}_1 d\bar{r}_2 d\bar{r}_3 \varrho^1(\bar{X}_1) \varrho^2(\bar{X}_2) \varrho^3(\bar{X}_3) V_{23}(\bar{r}_2 - \bar{r}_1, \bar{r}_3 - \bar{r}_1) \\
\langle V_{3N}^{\text{HF,1x}} \rangle = -\text{Tr}_1 \text{Tr}_2 \text{Tr}_3 \int d\bar{r}_1 d\bar{r}_2 d\bar{r}_3 \varrho^1(\bar{X}_3, \bar{X}_1) \varrho^2(\bar{X}_2) \varrho^3(\bar{X}_1, \bar{X}_3) V_{23}(\bar{r}_2 - \bar{r}_1, \bar{r}_3 - \bar{r}_1) P_{13}^{\tau\tau} + \frac{1}{2} \text{Tr}_1 \text{Tr}_2 \text{Tr}_3 \int d\bar{r}_1 d\bar{r}_2 d\bar{r}_3 \varrho^1(\bar{X}_1) \varrho^2(\bar{X}_3, \bar{X}_2) \varrho^3(\bar{X}_2, \bar{X}_3) V_{23}(\bar{r}_2 - \bar{r}_1, \bar{r}_3 - \bar{r}_1) P_{23}^{\tau\tau} \\
\langle V_{3N}^{\text{HF,2x}} \rangle = \text{Tr}_1 \text{Tr}_2 \text{Tr}_3 \int d\bar{r}_1 d\bar{r}_2 d\bar{r}_3 \varrho^1(\bar{X}_2, \bar{X}_1) \varrho^2(\bar{X}_3, \bar{X}_2) \varrho^3(\bar{X}_1, \bar{X}_3) V_{23}(\bar{r}_2 - \bar{r}_1, \bar{r}_3 - \bar{r}_1) P_{12}^{\tau\tau} P_{23}^{\tau\tau} 
\]
\[ \mathcal{E}^{CRA,2x} = \int d\vec{r} \left\{ C_{ijk}^3 \rho_0^3(\vec{r}) + C_{ijk}^1 \rho_0^1(\vec{r}) \rho_0(\vec{r}) + C_{ijk}^2 \rho_0^1(\vec{r}) \rho_1(\vec{r}) \rho_1(\vec{r}) + C_{ijk}^0 \rho_0(\vec{r}) \rho_1(\vec{r}) \rho_1(\vec{r}) \right. \\
+ C_{ijk}^1 \rho_0(\vec{r}) \rho_0^1(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) \rho_1(\vec{r}) \rho_1(\vec{r}) + C_{ijk}^2 \rho_0^1(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) \rho_1(\vec{r}) + C_{ijk}^3 \rho_0^1(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) \rho_1(\vec{r}) \rho_0^1(\vec{r}) \\
+ C_{ijk}^0 \rho_0(\vec{r}) \rho_0^1(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) \rho_1(\vec{r}) \rho_1(\vec{r}) + C_{ijk}^1 \rho_0(\vec{r}) \rho_0^1(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) \rho_1(\vec{r}) + C_{ijk}^2 \rho_0^1(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) \rho_1(\vec{r}) + C_{ijk}^3 \rho_0^1(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) \rho_1(\vec{r}) \\
+ C_{ijk}^0 \rho_0(\vec{r}) \rho_0^1(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) \rho_1(\vec{r}) + C_{ijk}^1 \rho_0(\vec{r}) \rho_0^1(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) + C_{ijk}^2 \rho_0^1(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) + C_{ijk}^3 \rho_0^1(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) \\
+ \left. C_{ijk}^0 \rho_0(\vec{r}) \rho_0^1(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) + C_{ijk}^1 \rho_0(\vec{r}) \rho_0^1(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) + C_{ijk}^2 \rho_0^1(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) + C_{ijk}^3 \rho_0^1(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_0(\vec{r}) \rho_1(\vec{r}) \right\}.
\]

+ 4 other classes of similar terms

Looks ugly (or beautiful, depending on your view), but a regular structure emerges:

\[ C^{ijk}[u] \xi_i \xi_j \xi_k , \quad u \equiv \frac{k_F(R)}{m_\pi} \quad \text{(note: u is NOT small)} \]

\[ C^{ijk}[u] = C_1^{ijk}[u] + C_2^{ijk}[u] \ln(1 + 4u^2) + C_3^{ijk}[u] \arctan(2u), \]

\[ C^{ijk}_{\alpha \beta}[u] = \text{polynomial} \]
Accuracy of the NVDME - Scalar exchange

\[ F_{s,exch}(R, r) = \int d\Omega_r \rho_q(r_1, r_2)\rho_q(r_2, r_1) \]

- Scalar NVDME works pretty good for exchange
- What about spin-vector piece?
Accuracy of the NVDME - Vector exchange

\[ \int d\Omega_r \mathbf{s}_n(r_1, r_2) \cdot \mathbf{s}_n(r_2, r_1) \]

- NVDME neglects 2 key aspects of finite fermi systems
  - anisotropy of local momentum distribution at the surface
  - diffuseness of local momentum distribution at the surface
Improved Vector DME

\[ \int d\Omega_r \mathbf{s}_n(r_1, r_2) \cdot \mathbf{s}_n(r_2, r_1) \]

- Modified DME ("PI-DME") to include \( n(k,R) \) surface anisotropy and diffuseness effects appropriate for finite fermi systems
• Inclusion of finite fermi phase space effects crucial for **quantitative** agreement
• Now completely parameter-free (compare vs. last year)
MSU (DME) plans for rest of Y3 and Y4

• Finish and submit the backlog of (~5) papers
  – NN and NNN DME couplings (2)
  – phase space averaged Pi-function DME improvements (1)
  – Mathematica (symbolic computational) tools (2)

• Validate Pi-function DME against exact HF
  – role of self-consistency, exact Hartree

• refit Skyrme + DME studies (w/ ORNL)
  – sensitivity studies & systematics
  – naturalness constraints for refits
  – higher gradients
  – different choices of $k_F\ (\tau\ and\ \nabla\ \rho\ dependence)$

• Extensions of the DME
  – pairing channel
  – beyond HF (proper treatment of dispersive effects via factorization/short-time methods)