

# MSU Year 4 Status Report



## I) Density Matrix Expansions

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II) In-medium SRG

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# $\label{eq:scopically-guided functionals} \mbox{-} V_{NN} + V_{NNN} + MBPT + DME \mbox{ to guide next-generation EDFs}$

# In-medium similarity renormalization group (IM-SRG)

- new ab-initio method
- effective interactions

## DME Year 4 Deliverables

- DME E<sub>x</sub>[ρ] from chiral EFT NN + NNN thru NNLO delivered to ORNL EDF group
  - Mathematica package + Python scripts available to public
  - Original NV-DME or PSA-DME options (others easy to implement)
  - Implemented in HFTHO and HFBRAD and 1st optimizations begun by ORNL group (Stoitsov, Kortelainen)
- Use improved DME to validate against ab-initio
  - 1st results obtained for neutron droplets w/Minnesota NN potential
  - Beyond HF and more realistic NN + NNN rest of Year 4 and 5
- Year 5 roadmap
  - revisit comparison to ab initio for nuclei w/realistic NN + NNN (DME improvements + exact Hartree)
  - microscopic constraints on short-range non-analytic density dependencies  $(\rho^{2+\gamma} \text{ etc.})$
  - comparison to OEP for  $E_x$

#### DME-related papers completed in Year 4

- "Microscopically-constrained Fock energy density functionals from chiral effective field theory. I. Two-nucleon interactions"
   B. Gebremariam, S. K. Bogner and T. Duguet arXiv:1003.5210 [nucl-th] SPIRES entry
- "Symbolic Integration Of A Product Of Two Spherical Bessel Functions With An Additional Exponential And Polynomial Factor"
   B. Gebremariam, T. Duguet and S. K. Bogner
   Comput. Phys. Commun. 181, 1136 (2010) SPIRES entry
- "Symbolic computation of the Hartree-Fock energy from a chiral EFT three-nucleon interaction at N<sup>2</sup>LO"
   B. Gebremariam, S. K. Bogner and T. Duguet Comput. Phys. Commun. 181, 1167 (2010) [arXiv:0912.3086 [physics.comp-ph]] SPIRES entry
- "An improved density matrix expansion for spin-unsaturated nuclei," B. Gebremariam, T. Duguet and S. K. Bogner, arXiv:0910.4979 [nucl-th] SPIRES entry

#### and 1 Ph.D. thesis (Biruk Gebremariam)

What could be missing in phenomenological EDFs?

- Density dependencies too simplistic
- Isovector components not well constrained
- What's the connection to many-body forces?

Turn to microscopic many body theory for guidance, aided by the simplifications enabled by soft RG-evolved interactions

Simplest idea: Map non-local exchange energy into local EDF (non-trivial density-dependence)

Density Matrix Expansion Revisited (Negele and Vautherin)

Expand of DM in local operators w/factorized non-locality

$$\langle \Phi | \psi^{\dagger} \left( \mathbf{R} - \frac{1}{2} \mathbf{r} \right) \psi \left( \mathbf{R} + \frac{1}{2} \mathbf{r} | \Phi \right) = \sum_{n} \prod_{n} (k_{F} r) \langle \mathcal{O}_{n}(\mathbf{R}) \rangle$$
$$\langle \mathcal{O}_{n}(\mathbf{R}) \rangle = \left[ \rho(\mathbf{R}), \nabla^{2} \rho(\mathbf{R}), \tau(\mathbf{R}), \mathbf{J}(\mathbf{R}), \ldots \right]$$
 NV, PSA, ...

Dependence on local densities/currents now manifest

$$\langle V_2 \rangle \sim \sum_{n,m} \int d\mathbf{R} \, \mathcal{O}_n(\mathbf{R}) \, \mathcal{O}_m(\mathbf{R}) \, \int d\mathbf{r} \, \Pi_n(k_F r) \Pi_m(k_F r) V_2(r) \\ \sim \sum_t \int d\mathbf{R} \left\{ C_t^{\rho\rho} \rho_t^2 + C_t^{\rho\tau} \rho_t \tau_t + C_t^{\rho\Delta\rho} \rho_t \Delta \rho_t + C_t^{JJ} \mathbf{J}_t^2 + C_t^{J\nabla\rho} \mathbf{J}_t \nabla \rho_t \cdots \right\}$$

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

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

$$C^{ij}[u] = \text{ rational polynomial}$$

#### Similarly for <V<sub>NNN</sub>> (but trilinear and many more terms...)

$$\begin{split} \mathcal{E}^{CR4,2x} &= \int d\vec{r} \left\{ \mathcal{C}_{7}^{\rho_{0}^{3}} \rho_{0}^{3}(\vec{r}) + \mathcal{C}_{7}^{\rho_{0}\rho_{1}^{2}} \rho_{0}(\vec{r}) \rho_{1}^{2}(\vec{r}) + \mathcal{C}_{7}^{\rho_{0}\rho_{1}c_{1}^{1}} \rho_{0}(\vec{r}) \rho_{1}(\vec{r}) \Delta\rho_{1}(\vec{r}) + \mathcal{C}_{7}^{\rho_{0}^{2}c_{0}^{2}} \rho_{0}^{2}(\vec{r}) \varsigma_{0}^{2}(\vec{r}) \\ &+ \mathcal{C}_{7}^{\rho_{0}^{2}c_{0}^{2}} \rho_{0}^{2}(\vec{r}) \zeta_{0}^{2}(\vec{r}) + \mathcal{C}_{7}^{\rho_{0}\rho_{1}c_{1}^{2}} \rho_{0}(\vec{r}) \rho_{1}(\vec{r}) \Delta\rho_{1}(\vec{r}) + \mathcal{C}_{7}^{\rho_{0}^{2}c_{0}^{2}} \rho_{0}^{2}(\vec{r}) \zeta_{0}^{2}(\vec{r}) \\ &+ \mathcal{C}_{7}^{\rho_{1}^{2}c_{0}^{2}} \rho_{1}^{2}(\vec{r}) \zeta_{0}^{2}(\vec{r}) + \mathcal{C}_{7}^{\rho_{0}\rho_{1}c_{1}^{2}} \rho_{0}(\vec{r}) \rho_{1}(\vec{r}) \zeta_{1}^{2}(\vec{r}) + \mathcal{C}_{7}^{\rho_{0}^{2}c_{0}^{2}} \rho_{0}^{2}(\vec{r}) \zeta_{1}^{1}(\vec{r}) \\ &+ \mathcal{C}_{7}^{\rho_{0}J_{0}^{2}} \rho_{0}(\vec{r}) J_{0}(\vec{r}) \cdot J_{0}(\vec{r}) + \mathcal{C}_{7}^{\rho_{1}J_{0}J_{1}} \rho_{1}(\vec{r}) J_{1}(\vec{r}) \nabla \vec{v} J_{0}(\vec{r}) + \mathcal{C}_{7}^{\rho_{1}J_{0}} \rho_{0}(\vec{r}) J_{1}(\vec{r}) \zeta_{1}^{1}(\vec{r}) \\ &+ \mathcal{C}_{7}^{2} \zeta_{0}^{2}J_{0} J_{0}(\vec{r}) \zeta_{1}(\vec{r}) \vec{v} \zeta_{1}^{2}(\vec{r}) + \mathcal{C}_{7}^{2} \zeta_{0}^{2}c_{0}^{2}(\vec{r}) J_{0}(\vec{r}) \zeta_{1}(\vec{r}) + \mathcal{C}_{7}^{\rho_{0}J_{1}} \zeta_{1}(\vec{r}) \vec{v} \zeta_{1}(\vec{r}) \zeta_{1}(\vec{r}) \\ &+ \mathcal{C}_{7}^{2} \zeta_{0}\rho_{0}(\vec{r}) J_{0}(\vec{r}) \zeta_{0}(\vec{r}) + \mathcal{C}_{7}^{2} \zeta_{0}^{2}c_{0}^{2}(\vec{r}) J_{0}(\vec{r}) \zeta_{0}(\vec{r}) + \mathcal{C}_{7}^{2} \zeta_{0}^{2}c_{0}^{2}(\vec{r}) J_{0}(\vec{r}) \zeta_{0}(\vec{r}) \\ &+ \mathcal{C}_{7}^{2} \zeta_{0}\rho_{0}J_{0} \nabla J_{0} \nabla J_{0}(\vec{r}) \vec{\nabla} \zeta_{0}(\vec{r}) + \mathcal{C}_{7}^{2} \zeta_{0}^{2}c_{0}^{2}(\vec{r}) J_{0}(\vec{r}) \zeta_{0}(\vec{r}) \zeta_{0}(\vec{r}) \\ &+ \mathcal{C}_{7}^{2} \zeta_{0}\rho_{0}J_{0} \zeta_{0} \zeta_{0} \vec{r}) \zeta_{0}(\vec{r}) \zeta_{0} \vec{r} \\ &+ \mathcal{C}_{7}^{2} \zeta_{0}J_{0}} \zeta_{0}(\vec{r}) \zeta_{0}(\vec{r}) \zeta_{0} \vec{r} \\ &+ \mathcal{C}_{7}^{2} \zeta_{0}J_{0} \zeta_{0}(\vec{r}) \zeta_{0}(\vec{r}) \zeta_{0} \vec{r}) \zeta_{0}(\vec{r}) \zeta_{0} \vec{r} \\ &+ \mathcal{C}_{7}^{2} \zeta_{0}J_{0} \zeta_{0} \zeta_{0} \vec{r}) \zeta_{0}(\vec{r}) \zeta_{0} \vec{r} \\ &+ \mathcal{C}_{7}^{2} \zeta_{0}J_{0} \zeta_{0} \vec{r} \\ &+ \mathcal{C}_{7}^{2} \zeta_{0}J_{0} \vec{r} \\ &+ \mathcal{C}_{7}^{2} \zeta_{0} \zeta_{0} \vec{r} \\ &+ \mathcal{C}_{7}^{2}$$

$$\begin{split} C^{ijk}[u]\xi_i\xi_j\xi_k \ , \quad u \equiv \frac{k_F(R)}{m_\pi} \quad \text{(note: u is NOT small)} \\ C^{ijk}[u] = C_1^{ijk}[u] + C_2^{ijk}[u] \ln(1 + 4u^2) + C_3^{ijk}[u] \arctan(2u), \\ C^{ijk}_{\alpha}[u] = \text{rational polynomial} \end{split}$$

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#### New development: DME for chiral NNN force (N2LO)

• Expect interesting spin-orbit/tensor couplings from TPE   

$$V_c(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) \sim \frac{\sigma_1 \cdot \mathbf{q}_1 \sigma_2 \cdot \mathbf{q}_2}{(q_1^2 + m_\pi^2)(q_2^2 + m_\pi^2)} F_{123}^{\alpha\beta} \tau_1^{\alpha} \tau_2^{\beta} + perms$$
  
 $F_{123}^{\alpha\beta} \equiv \delta_{\alpha\beta} \left[ -4 \frac{c_1 m_\pi^2}{f_\pi^2} + 2 \frac{c_3}{f_\pi^2} \mathbf{q}_1 \cdot \mathbf{q}_2 \right] + \frac{c_4}{f_\pi^2} \epsilon^{\alpha\beta\gamma} \tau_3^{\gamma} \sigma_3 \cdot (\mathbf{q}_1 \times \mathbf{q}_2)$ 

Empirical EDFs (Skyrme, Gogny,...) spin-orbit coupling is density independent => appropriate for NN spin-orbit forces (short range)

This is a mismatch since microscopic NNN interactions are long-range (DME ==> density dependent  $J \cdot \nabla \rho$  couplings)

### Prescriptions for $\Pi_n$ -functions

Phase space averaging (PSA-DME) (Gebremariam et al. arXiv:0910.4979)

$$\rho(\vec{r}_1, \vec{r}_2) = e^{i\vec{r}\cdot\vec{k}} e^{\frac{\vec{r}}{2}\cdot(\nabla_1 - \nabla_2) - i\vec{r}\cdot\vec{k}} \rho(\vec{r}_1, \vec{r}_2) \bigg|_{\vec{r}_1 = \vec{r}_2 = \vec{R}}$$

Average the non-locality operator over local momentum distribution  $g(\mathbf{R},\mathbf{k})$  and expand exponentiated gradients

$$\rho(\vec{r}_1, \vec{r}_2) \approx \int d^3 \vec{k} \ g(\vec{R}, \vec{k}) \ e^{i\vec{k}\cdot\vec{r}} \sum_{n=0}^2 \frac{1}{n!} \left\{ \vec{r} \cdot \left( \frac{\nabla_1 - \nabla_2}{2} - i\vec{k} \right) \right\}^n \left. \rho(\vec{r}_1, \vec{r}_2) \right|_{\vec{r}_1 = \vec{r}_2 = \vec{R}}$$

Easy to build in physics associated with surface effects in finite fermi systems (non-isotropic g(R,k))

#### Crucial to accurately describe spin-vector part of OBDM

## Prescriptions for $\Pi_n$ -functions

Negele and Vautherin (NV-DME)

Truncated Bessel expansion of non-locality operator **Sufficient for spin-unsaturated nuclei only** 



Why it fails: no phase space averaging (not even over INM) done for spin-vector part



Look at  $\int d\mathbf{r} \, d\mathbf{R} \, V_{1\pi}(r) \, \mathbf{s}_n(\mathbf{r}_1, \mathbf{r}_2) \cdot \mathbf{s}_n(\mathbf{r}_2, \mathbf{r}_1)$ 



Inclusion of finite fermi phase space effects crucial for quantitative agreement
completely parameter-free

Can now apply modified DME with confidence to spin-unsaturated systems

Including Long Range Chiral EFT in Skyrme-like EDFs

$$V_{EFT} = V_{ct}(\Lambda) + V_{1\pi} + V_{2\pi} + \cdots$$

Each HF DME coupling function splits into 2 terms

- 1) Skyrme-like coupling constants (contact terms)
- 2) Nontrivial coupling **functions** from "universal" pion physics

$$C_t^{\rho\tau} \Rightarrow C_t^{\rho\tau}(\Lambda; V_{ct}) + C_t^{\rho\tau}[k_F(\mathbf{R}); V_{\pi}]$$
 Etc...

From contact terms in EFT/RG V's

From pion exchanges

Suggests a microscopically-improved Skyrme phenomenology

Add pion-exchange couplings to existing Skyrme EDF and refit Skyrme constants (mimics higher-order ladder contributions)

Analogous to separation of long- and short-distance Coulomb (J. Drut's talk)

#### Including DME pion couplings in Skyrme



	SVD Optimization Results				
$\chi^2$	12.5002	2.1235	1.837	1.7662	1.7884
RMSD(E)	7.008	2.6931	2.5539	2.5143	2.590
$RMSD(\Delta_n)$	0.1297	0.0828	0.0587	0.0554	0.0476
$RMSD(\Delta_p)$	0.094	0.0988	0.0902	0.0866	0.0706

See Mario/Markus's talk for details of the implementation and restricted "pre-optimization" fits.

Implemented into HFTHO and HFBRAD
 Stable enough for optimization

3) Bulk properties ok (as expected)

4) Small but stable improvement over Skyrme

#### No show stoppers yet!

\* 1st paper by ORNL group + MSU & OSU coming soon

# Part 2: In-medium SRG



In-medium similarity renormalization group (IM-SRG)

- new ab-initio method
- effective interactions

See arXiv:1006.3639

#### The Similarity Renormalization Group Wegner, Glazek and Wilson

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  $\lambda => 0$ 

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

$$\lambda \equiv s^{-1/4}$$

 $\mathcal{G}_{\lambda} = T \Rightarrow H_{\lambda}$  driven towards diagonal in k – space  $\mathcal{G}_{\lambda} = PH_{\lambda}P + QH_{\lambda}Q \Rightarrow H_{\lambda}$  driven to block-diagonal

increases "perturbativeness", accelerates basis expansions, ...

need to evolve NNN (at least) to keep  $\lambda$  independent A > 2 observables (E. Jurgenson's talk)

# 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) :

$$\begin{split} H &= E_{vac} + \sum f_i N(a_i^{\dagger} a_i) + \frac{1}{4} \sum \Gamma_{ijkl} N(a_i^{\dagger} a_j^{\dagger} a_l a_k) + \frac{1}{36} \sum W_{ijklmn} N(a_i^{\dagger} a_j^{\dagger} a_k^{\dagger} a_n a_m a_l) \\ E_{vac} &= \langle \Phi | H | \Phi \rangle \\ f_i &= t_{ii} + \sum_h \langle ih | V_2 | ih \rangle n_h + \frac{1}{2} \sum_{hh'} \langle ihh' | V_3 | ihh' \rangle n_h n_{h'} \\ \Gamma_{ijkl} &= \langle ij | V_2 | kl \rangle + \sum_h \langle ijh | V_3 | klh \rangle n_h \\ W_{ijklmn} &= \langle ijk | V_3 | lmn \rangle \qquad \langle \Phi | N(\cdots) | \Phi \rangle = 0 \end{split}$$

0-, 1-, 2-body terms contain some 3NF effects thru density dependence => Efficient truncation scheme for evolution of 3N?

#### In-medium SRG for Nuclear matter

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

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

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

Microscopic realization of SM ideas: dominant MF + weak A-dependent NN<sub>eff</sub>

### Correlations "adiabatically" summed into $H(\lambda)$



\*Neglects ph-channel. See Heiko Hergert's talk.

#### In-medium SRG to diagonalize closed-shell nuclei

Define "offdiagonal" as terms that don't annihilate the reference HF state

$$\Gamma^{od}(s) = \sum_{pp'hh'} \Gamma_{pp'hh'}(s) \{a_p^{\dagger} a_{p'}^{\dagger} a_h a_{h'}\} + h.c.$$
  
$$\eta(s) = [H(s), H \quad (s)]$$
  
$$f^{od}(s) = \sum_{ph} f_{ph}(s) \{a_p^{\dagger} a_h\} + h.c.,$$

HF reference state decouples from higher npnh states

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

 $\lambda \equiv s^{-1/4}$ 

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

where  $P = |\Phi\rangle \langle \Phi|$  and Q = 1 - P.

### IM-SRG(2) diagonalization of closed-shell systems



Comparable to coupled-cluster in closed shell nuclei.

Neutron droplet comparisons in rest of year 4



Similar scaling with number of orbitals  $\sim N^6$ 

# Can also use IM-SRG(2) to "soften" convergence of MBPT well before total decoupling achieved



Note the  $\sim$  cutoff-independent CC results using H(s). Further indication that our N-ordered truncation is robust.

#### Some observations

- pp channel + 2 ph channels treated on equal footing (like Parquet theory but without the technical problems of energy-dependence, poles, etc.)
- 2) Intrinsically non-perturbative, and issues of small energy denominators, poles, etc. bypassed.
- 3) no unlinked diagrams (size extensive, etc.)

4) "3rd-order exact" and similar scaling to coupled cluster (deeper connection?)

5) Extensions to open shell possible (derive valence Heff)

1) Eliminate quasi-particle number changing interactions

$$\eta = [Q, H(s)] , Q = \sum_{i} sgn(\epsilon_{i} - \epsilon_{F}) \{a_{i}^{\dagger}a_{i}\}$$



non-perturbatively derive valence shell-model Heff/Oeff

2) Decouple highly-virtual s.p. orbitals

$$\eta = [Q, H(s)] , Q = \sum_{i} \theta(\epsilon_i - (\epsilon_F + \Lambda) \{a_i^{\dagger} a_i\}$$



Evolved  $H(\infty)$  doesn't mix many-body states that differ in the number of s.p. orbits above the chosen cutoff

# use to truncate # of basis states for ab-initio calculation of low-lying states

3) Decouple highly-virtual and deeply bound s.p. orbitals

$$\eta = [Q, H(s)] , Q = \sum_{i} \theta(|\epsilon_i - \epsilon_F| - \Lambda) \{a_i^{\dagger} a_i\}$$



Evolved  $H(\infty)$  doesn't mix many-body states that differ in the # of s.p. orbits lying within the cutoff centered on the fermi level

# reduce d.o.f. to just a few active orbitals close to the fermi level (i.e., shell model)

4) IM-SRG for infinite matter (See Heiko's talk)

- include particle-hole channel (hard!!)
  - is it worth the effort? Folklore about ph-contributions to bulk...
- Use HFB groundstate to N-order w.r.t.
  - bypass technical problems of Nambu-Gorkov Green's functions?